# Many Body Quantum Mechanics

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# Contents

# 1 Preliminaries: Hilbert Spaces and Operators

The basic mathematical objects in quantum mechanics are Hilbert spaces and operators defined on them. In order to fix notations we briefly review the definitions.

**DEFINITION 1.1** (Hilbert Space)**.** A Hilbert Space $\mathcal{H}$ is a vector space endowed with a sesquilinear map $(\cdot,\cdot) : \mathcal{H}\times\mathcal{H}\to\mathbb{C}$ (i.e., a map which is conjugate linear in the first variable and linear in the second[1]) such that $\|\phi\| = (\phi,\phi)^{1/2}$ defines a norm on $\mathcal{H}$ which makes $\mathcal{H}$ into a complete metric space.

*REMARK* 1.2. We shall mainly use the following two properties of Hilbert spaces.

(a) To any closed subspace $V\subset\mathcal{H}$ there corresponds the orthogonal complement $V^\perp$ such that $V\oplus V^\perp = \mathcal{H}$.

(b) Riesz representation Theorem: To any continuous linear functional $\Lambda : \mathcal{H}\to\mathbb{C}$ there is a unique $\psi\in\mathcal{H}$ such that $\Lambda(\phi) = (\psi,\phi)$ for all $\phi\in\mathcal{H}$.

We denote by $\mathcal{H}^*$ the dual of the Hilbert space $\mathcal{H}$, i.e., the space of all continuous linear functionals on $\mathcal{H}$. The map $J:\mathcal{H}\to\mathcal{H}^*$ defined by $J(\psi)(\phi) = (\psi,\phi)$ is according to Riesz representation Theorem an anti-linear isomorphism. That $J$ is anti-linear (or conjugate-linear) means that $J(\alpha\phi+\beta\psi) = \overline{\alpha}J(\phi)+\overline{\beta}J(\psi)$ for $\alpha,\beta\in\mathbb{C}$ and $\phi,\psi\in\mathcal{H}$.

We shall always assume that our Hilbert spaces are separable and therefore that they have countable orthonormal bases.

We will assume that the reader is familiar with elementary notions of measure theory, in particular the fact that $L^2$- spaces are Hilbert spaces.

**DEFINITION 1.3** (Operators on Hilbert spaces)**.** By an operator (or more precisely densely defined operator) $A$ on a Hilbert space $\mathcal{H}$ we mean a linear map $A : D(A)\to\mathcal{H}$ defined on a *dense* subspace $D(A)\subset\mathcal{H}$. Dense refers to the fact that the norm closure $\overline{D(A)} = \mathcal{H}$.

**DEFINITION 1.4** (Extension of operator)**.** If $A$ and $B$ are two operators such that $D(A)\subseteq D(B)$ and $A\phi = B\phi$ for all $\phi\in D(A)$ then we write $A\subset B$ and say that $B$ is an *extension* of $A$.

[1] This is the convention in physics. In mathematics the opposite convention is used.

Note that the domain is part of the definition of the operator. In defining operators one often starts with a domain which turns out to be too small and which one then later extends.

**DEFINITION 1.5** (Symmetric operator)**.** We say that $A$ is a *symmetric operator* if

$$(\psi, A\phi) = (A\psi, \phi) \tag{1}$$

for all $\phi, \psi \in D(A)$.

The result in the following problem is of great importance in quantum mechanics.

**PROBLEM 1.6.** *Prove that (1) holds if and only if $(\psi, A\psi) \in \mathbb{R}$ for all $\psi \in D(A)$.*

*REMARK* 1.7. It is in general not easy to define the sum of two operators $A$ and $B$. The problem is that the natural domain of $A + B$ would be $D(A) \cap D(B)$, which is not necessarily densely defined.

*EXAMPLE* 1.8. The Hilbert space describing a one-dimensional particle without internal degrees of freedom is $L^2(\mathbb{R})$, the space of square (Lebesgue) integrable functions defined modulo sets of measure zero. The inner product on $L^2(\mathbb{R})$ is given by

$$(g, f) = \int_{\mathbb{R}} \overline{g(x)} f(x)\, dx.$$

The operator describing the kinetic energy is the second derivative operator. $A = -\frac{1}{2}\frac{d^2}{dx^2}$ defined originally on the subspace

$$D(A) = C_0^2(\mathbb{R}) = \left\{ f \in C^2(\mathbb{R}) : f \text{ vanishes outside a compact set } \right\}.$$

Here $C^2(\mathbb{R})$ refers to the twice continuously differentiable functions on the real line. The subscript 0 refers to the compact support.

The operator $A$ is symmetric, since for $\phi, \psi \in D(A)$ we have by integration by parts

$$\begin{aligned}(\psi, A\phi) &= -\frac{1}{2}\int_{\mathbb{R}} \overline{\psi(x)} \frac{d^2\phi}{dx^2}(x) dx \\ &= \frac{1}{2}\int_{\mathbb{R}} \overline{\frac{d\psi}{dx}(x)} \frac{d\phi}{dx}(x) dx = -\frac{1}{2}\int_{\mathbb{R}} \overline{\frac{d^2\psi}{dx^2}(x)} \phi(x) dx = (A\psi, \phi).\end{aligned}$$

**DEFINITION 1.9** (Bounded operators)**.** An operator $A$ is said to be *bounded* on the Hilbert Space $\mathcal{H}$ if $D(A) = \mathcal{H}$ and $A$ is continuous, which by linearity is equivalent to

$$\|A\| = \sup_{\phi,\ \|\phi\|=1} \|A\phi\| < \infty.$$

The number $\|A\|$ is called the norm of the operator $A$. An operator is said to be *unbounded* if it is not bounded.

**PROBLEM 1.10.** *(a) Show that if an operator $A$ with dense domain $D(A)$ satisfies $\|A\phi\| \leq M\|\phi\|$ for all $\phi \in D(A)$ for some $0 \leq M < \infty$ then $A$ can be uniquely extended to a bounded operator.*

*(b) Show that the kinetic energy operator $A$ from Example 1.8 cannot be extended to a bounded operator on $L^2(\mathbb{R})$.*

**DEFINITION 1.11** (Adjoint of an operator)**.** If $A$ is an operator we define the adjoint $A^*$ of $A$ to be the linear map $A^* : D(A^*) \to \mathcal{H}$ defined on the space

$$D(A^*) = \left\{ \phi \in \mathcal{H} \;\middle|\; \sup_{\psi \in D(A),\ \|\psi\|=1} |(\phi, A\psi)| < \infty \right\}$$

and with $A^*\phi$ defined such that

$$(A^*\phi, \psi) = (\phi, A\psi)$$

for all $\psi \in D(A)$. The existence of $A^*\phi$ for $\phi \in D(A^*)$ is ensured by the Riesz representation Theorem (why?). If $D(A^*)$ is dense in $\mathcal{H}$ then $A^*$ is an operator on $\mathcal{H}$.

**PROBLEM 1.12.** *Show that the adjoint of a bounded operator is a bounded operator.*

**PROBLEM 1.13.** *Show that $A$ is symmetric if and only if $A^*$ is an extension of $A$, i.e., $A \subset A^*$.*

*EXAMPLE* 1.14 (Hydrogen atom)*.* One of the most basic examples in quantum mechanics is the hydrogen atom. In this case the Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^3; \mathbb{C}^2)$, i.e., the square integrable functions on $\mathbb{R}^3$ with values in $\mathbb{C}^2$. Here $\mathbb{C}^2$ represents the internal spin degrees of freedom. The inner product is

$$(g, f) = \int_{\mathbb{R}^3} g(x)^* f(x)\, dx,$$

The total energy operator is[2]

$$H = -\tfrac{1}{2}\Delta - \frac{1}{|x|}, \tag{2}$$

where $\Delta = \partial_1^2 + \partial_2^2 + \partial_3^2$, is the Laplacian. I.e.,

$$(H\phi)(x) = -\tfrac{1}{2}\Delta\phi(x) - \frac{1}{|x|}\phi(x)$$

The domain of $H$ may be chosen to be

$$\begin{aligned} D(H) &= C_0^2\left(\mathbb{R}^3; \mathbb{C}^2\right) \qquad (3) \\ &= \left\{ f \in C^2(\mathbb{R}^3; \mathbb{C}^2) : f \text{ vanishes outside a compact subset of } \mathbb{R}^3 \right\}. \end{aligned}$$

It is easy to see that if $\phi \in D(H)$ then $H\phi \in \mathcal{H}$. It turns out that one may extend the domain of $H$ to the Sobolev space $H^2(\mathbb{R}^3)$. We will return to this later.

*EXAMPLE* 1.15 (Schrödinger operator). We may generalize the example of hydrogen to operators on $L^2(\mathbb{R}^n)$ or $L^2(\mathbb{R}^n; \mathbb{C}^q)$ of the form

$$-\tfrac{1}{2}\Delta - V(x)$$

where $V : \mathbb{R}^n \to \mathbb{R}$ is a potential. If $V$ is a locally square integrable function we may start with the domain $C_0^2\left(\mathbb{R}^n\right)$ or $C_0^2\left(\mathbb{R}^n; \mathbb{C}^2\right)$. We shall return to appropriate conditions on $V$ later. We call an operator of this form a Schrödinger operator. See Section 5

Correction since August 30, 09: $V \to -V$ to agree with Definition 5.1.

**DEFINITION 1.16** (Compact, trace class, and Hilbert-Schmidt operators). A linear operator $K$ is said to be a *compact operator* on a Hilbert space $\mathcal{H}$ if $D(K) = \mathcal{H}$ and there are orthonormal bases $u_1, u_2, \ldots$ and $v_1, v_2, \ldots$ for $\mathcal{H}$ and a sequence $\lambda_1, \lambda_2, \ldots$ with $\lim_{n\to\infty} \lambda_n = 0$ such that

$$K\phi = \sum_{n=1}^{\infty} \lambda_n (u_n, \phi) v_n \tag{4}$$

for all $\phi \in \mathcal{H}$. A compact operator $K$ is said to be *trace class* if $\sum_{n=1}^{\infty} |\lambda_n| < \infty$ and it is called *Hilbert-Schmidt* if $\sum_{n=1}^{\infty} |\lambda_n|^2 < \infty$.

If $K$ is trace class the *trace of* $K$ is defined to be

$$\mathrm{Tr} K = \sum_{n=1}^{\infty} \lambda_n (u_n, v_n).$$

[2] We use units in which Planck's constant $\hbar$, the electron mass $m_{\mathrm{e}}$, and the electron charge $e$ are all equal to unity

**PROBLEM 1.17.** *(a) Show that a trace class operator is Hilbert-Schmidt.*

*(b) Show that the trace of a trace class operator on a Hilbert space $\mathcal{H}$ is finite and that if $\phi_1, \phi_2, \ldots$ is any orthonormal basis for $\mathcal{H}$ and $K$ is any trace class operator on $\mathcal{H}$ then*

$$\mathrm{Tr}K = \sum_{n=1}^{\infty} (\phi_n, K\phi_n).$$

**PROBLEM 1.18.** *(a)* **(Super symmetry)** *Show that if $K$ is a compact operator then $K^*K$ and $KK^*$ have the same non-zero eigenvalues with the same (finite) multiplicities.*

*(b) Show that if $K$ is a compact operator then it maps the eigenspaces of $K^*K$ corresponding to non-zero eigenvalues to the eigenspace of $KK^*$ with the same eigenvalue.*

*(c)* **(Spectral Theorem for compact operators)** *Show that if $K$ is a compact symmetric operator on a Hilbert space $\mathcal{H}$ then there is an orthonormal basis $u_1, u_2, \ldots$ for $\mathcal{H}$ and a sequence $\lambda_1, \lambda_2, \ldots \in \mathbb{R}$ such that $\lim_{n\to\infty} \lambda_n = 0$ and*

$$K\phi = \sum_{n=1}^{\infty} \lambda_n (u_n, \phi) u_n.$$

*(Hint: Diagonalize the finite dimensional operator obtained by restricting $K$ to a non-zero eigenvalue eigenspace of $K^*K = K^2$.)*

## 1.1 Tensor products of Hilbert spaces

Let $\mathcal{H}$ and $\mathcal{K}$ be two Hilbert spaces. The tensor product of $\mathcal{H}$ and $\mathcal{K}$ is a Hilbert space denoted $\mathcal{H} \otimes \mathcal{K}$ together with a bilinear map

$$\mathcal{H} \times \mathcal{K} \ni (u, v) \mapsto u \otimes v \in \mathcal{H} \otimes \mathcal{K},$$

such that the inner products satisfy

$$(u_1 \otimes v_1, u_2 \otimes v_2)_{\mathcal{H}\otimes\mathcal{K}} = (u_1, u_2)_{\mathcal{H}} (v_1, v_2)_{\mathcal{K}},$$

and such that the $\mathrm{span}\{u \otimes v \,|\, u \in \mathcal{H}, v \in \mathcal{K}\}$ is dense in $\mathcal{H} \otimes \mathcal{K}$. We call the vectors of the form $u \otimes v$ for *pure tensor products*.

The tensor product is unique in the sense that if $\mathcal{H}\widehat{\otimes}\mathcal{K}$ is another tensor product then the map $u\widehat{\otimes}v \mapsto u\otimes v$ extends uniquely to an isometric isomorphism.

**PROBLEM 1.19.** *Prove the above uniqueness statement.*

If $(u_\alpha)_{\alpha\in I}$ is an orthonormal basis for $\mathcal{H}$ and $(v_\beta)_{\beta\in J}$ is an orthonormal basis for $\mathcal{K}$, then $(u_\alpha\otimes v_\beta)_{\alpha\in I\beta\in J}$ is an orthonormal basis for $\mathcal{H}\otimes\mathcal{K}$.

**PROBLEM 1.20** (Construction of the tensor product)**.** *Show that the tensor product $\mathcal{H}\otimes\mathcal{K}$ may be identified with the space $\ell^2(I\times J)$ and*

$$(u\otimes v)_{ij}=(u_i,u)_{\mathcal{H}}(v_j,v)_{\mathcal{K}}.$$

More generally, if $\mu$ is a $\sigma$-finite measure on a measure space $X$ and $\nu$ is a $\sigma$-finite measure on a measure space $Y$, it follows from Fubini's Theorem that the tensor product $L^2(X,\mu)\otimes L^2(Y,\nu)$ may be identified with $L^2(X\times Y,\mu\times\nu)$ (where $\mu\times\nu$ is the product measure) and

$$f\otimes g(x,y)=f(x)g(y).$$

**PROBLEM 1.21.** *Use Fubini's Theorem to show that $L^2(X\times Y,\mu\times\nu)$ in this way may be identified with $L^2(X,\mu)\otimes L^2(Y,\nu)$.*

If we have an operator $A$ on the Hilbert space $\mathcal{H}$ and an operator $B$ on the Hilbert space $\mathcal{K}$ then we may form the tensor product operator $A\otimes B$ on $\mathcal{H}\otimes\mathcal{K}$ with domain

$$D(A\otimes B)=\operatorname{span}\{\phi\otimes\psi\mid\phi\in D(A),\quad\psi\in D(B)\}$$

and acting on pure tensor products as

$$A\otimes B(\phi\otimes\psi)=(A\phi)\otimes(B\psi).$$

The tensor product may in a natural way be extended to more than two Hilbert spaces. In particular, we may for $N=1,2,\ldots$ consider the $N$-fold tensor product $\bigotimes^N\mathcal{H}$ of a Hilbert space $\mathcal{H}$ with itself. On this space we have a natural action of the symmetric group $S_N$. I.e., if $\sigma\in S_N$ then we have a unitary map $U_\sigma:\bigotimes^N\mathcal{H}\to\bigotimes^N\mathcal{H}$ defined uniquely by the following action on the pure tensor products

$$U_\sigma u_1\otimes\cdots\otimes u_N=u_{\sigma(1)}\otimes\cdots\otimes u_{\sigma(N)}.$$

We shall denote by $\mathrm{Ex}:\mathcal{H}\otimes\mathcal{H}\to\mathcal{H}\otimes\mathcal{H}$ the unitary corresponding to a simple interchange of the two tensor factors.

**PROBLEM 1.22.** *Show that $U_\sigma$ defines a unitary operator and that the two operators*

$$P_+ = (N!)^{-1}\sum_{\sigma\in S_N} U_\sigma, \quad P_- = (N!)^{-1}\sum_{\sigma\in S_N}(-1)^\sigma U_\sigma, \tag{5}$$

*are orthogonal projections ($P = P^*$, $P^2 = P$) satisfying $P_-P_+ = 0$ if $N \geq 2$. Here $(-1)^\sigma$ is the sign of the permutation $\sigma$.*

Correction since April 15: $N \geq 2$ added

Correction since May 3: definition of $(-1)^\sigma$ added

correction July 6: sentence corrected

The two projections $P_\pm$ define two important subspaces of $\bigotimes^N \mathcal{H}$.

**DEFINITION 1.23** (Symmetric and anti-symmetric tensor products)**.** The symmetric tensor product is the space

$$\bigotimes_{\text{sym}}^N \mathcal{H} := P_+\Big(\bigotimes^N \mathcal{H}\Big). \tag{6}$$

The antisymmetric tensor product is the space

$$\bigwedge^N \mathcal{H} := P_-\Big(\bigotimes^N \mathcal{H}\Big). \tag{7}$$

We define the antisymmetric tensor product of the vectors $u_1,\ldots,u_N \in \mathcal{H}$ as

$$u_1\wedge\cdots\wedge u_N = (N!)^{1/2}P_-(u_1\otimes\cdots\otimes u_N). \tag{8}$$

**PROBLEM 1.24.** *Show that if $u_1,\ldots,u_N$ are orthonormal then $u_1\wedge\cdots\wedge u_N$ is normalized (i.e., has norm 1).*

**PROBLEM 1.25.** *Let $u_1,\ldots,u_N$ be orthonormal functions in an $L^2$ space $L^2(X,\mu)$ over the measure space $X$ with measure $\mu$. Show that in the space $L^2(X^N,\mu^N)$*

$$u_1\wedge\cdots\wedge u_N(x_1,\ldots,x_N) = (N!)^{-1/2}\det\begin{pmatrix} u_1(x_1) & \cdots & u_N(x_1)\\ u_1(x_2) & \cdots & u_N(x_2)\\ & \vdots & \\ u_1(x_N) & \cdots & u_N(x_N)\end{pmatrix}.$$

*One refers to this as a Slater determinant.*

**PROBLEM 1.26.** *Show that if $\dim\mathcal{H} < N$ then $\bigwedge^N \mathcal{H} = \{0\}$.*

**PROBLEM 1.27.** *Let $X$ be a measure space with measure $\mu$ and let $\mathcal{H}$ be a Hilbert space. Show that we may identify the tensor product $L^2(X,\mu)\otimes\mathcal{H}$ with the Hilbert space $L^2(X,\mu;\mathcal{H})$ of $\mathcal{H}$-valued $L^2$ functions on $X$, where the tensor product of $f\in L^2(X,\mu)$ with $u\in\mathcal{H}$ is the function*

$$f\otimes u(x)=f(x)u.$$

# 2 The Principles of Quantum Mechanics

We shall here briefly review the principles of quantum mechanics. The reader with little or no experience in quantum mechanics is advised to also consult standard textbooks in physics.

In quantum mechanics a *pure* state of a physical system is described by a unit vector $\psi_0$ in a Hilbert space $\mathcal{H}$. The measurable quantities correspond to 'expectation values'

$$\langle A\rangle_{\psi_0}=(\psi_0,A\psi_0),$$

of operators $A$ on $\mathcal{H}$. Of course, in order for this to make sense we must have $\psi_0\in D(A)$. Since measurable quantities are real the relevant operators should have real expectation values, i.e, the operators are symmetric. (See Problem 1.6).

The physical interpretation of the quantity $\langle A\rangle_{\psi_0}$ is that it is the average value of 'many' measurements of the observable described by the operator $A$ in the state $\psi_0$.

As an example $\psi_0\in C_0^2(\mathbb{R}^3;\mathbb{C}^2)$ with $\int|\psi_0|^2=1$ may represent a state of a hydrogen atom (see Example 1.14). The average value of many measurements of the energy of the atom in this state will be

$$\begin{aligned}\left(\psi_0,(-\tfrac12\Delta-\frac{1}{|x|})\psi_0\right) &= \int_{\mathbb{R}^3}\psi_0(x)^*(-\tfrac12\Delta-\frac{1}{|x|})\psi_0(x)\,dx\\ &= \int_{\mathbb{R}^3}\tfrac12|\nabla\psi_0(x)|^2-\frac{1}{|x|}|\psi_0(x)|^2\,dx,\end{aligned}$$

where the last equality follows by integration by parts.

The general quantum mechanical state, which is not necessarily pure is a statistical average of pure states, i.e, expectations are of the form

$$\langle A\rangle=\sum_{n=1}^{\infty}\lambda_n(\psi_n,A\psi_n),\tag{9}$$

where $0 \leq \lambda_n \leq 1$ with $\sum_n \lambda_n = 1$ and $\psi_n$ is a family of orthonormal vectors. In this representation the $\lambda_n$ are unique (i.e. independent on the choice of $\{\psi_n\}$) [3].

How far the state is from being pure is naturally measured by its *entropy*.

Correction since April 15: unit $\to$ orthonormal. Uniqueness statement. Problem added to footnote

Correction since August 30, 09: explanation for the uniqueness of $\lambda_n$

**DEFINITION 2.1** (Von Neumann entropy)**.** The *von Neumann entropy* of a state $\langle\cdot\rangle$ of the form (9) is

$$S(\langle\cdot\rangle) = -\sum_{n=1}^{\infty} \lambda_n \log \lambda_n,$$

which is possibly $+\infty$. (We use the convention that $t \log t = 0$ if $t = 0$.)

Addition since April 15: which is possibly $+\infty$

Note that the entropy vanishes if and only if the state is pure.

Of particular interest are the *equilibrium states*, either zero (absolute) temperature or positive temperature states. The zero temperature state is usually a pure state, i.e., given by one vector, whereas the positive temperature states (the Gibbs states) are non-pure. Both the zero temperature states and the positive temperature states are described in terms of the energy operator, the Hamiltonian. We shall here mainly deal with the zero temperature equilibrium states, the *ground states*.

**DEFINITION 2.2** (Stability and Ground States)**.** Consider a physical system described by a Hamiltonian, i.e., energy operator, $H$ on a Hilbert space $\mathcal{H}$. If

$$\inf_{\phi\in D(H),\ \|\phi\|=1} (\phi, H\phi) > -\infty$$

the system is said to be stable. If this holds we call

$$E = \inf_{\phi\in D(H),\ \|\phi\|=1} (\phi, H\phi)$$

for the *ground state energy*.

A *ground state* for the system, if it exists, is a unit vector $\psi_0 \in D(H)$ such that

$$(\psi_0, H\psi_0) = \inf_{\phi\in D(H),\ \|\phi\|=1} (\phi, H\phi)\,.$$

Thus a ground state is characterized by minimizing the energy expectation.

Correction since April 15: stable added

**DEFINITION 2.3** (Free energy and temperature states)**.** The *free energy* of a stable system at temperature $T \geq 0$ is

$$F(T) = \inf_{\substack{\langle\cdot\rangle \\ \langle H\rangle<\infty}} \left(\langle H\rangle \ - TS(\langle\cdot\rangle)\right),$$

(possibly $-\infty$) where the infimum is over all states of the form (9) with $\psi_n \in D(H)$ for $n = 1, 2, \ldots$. If for $T > 0$ a minimizer exists for the free energy variation above it is called a Gibbs state at temperature $T$.

**PROBLEM 2.4.** *Show that $F(T)$ is a decreasing function of $T$ and that $F(0) = E$, i.e., the free energy at zero temperature is the ground state energy.*

**PROBLEM 2.5** (Ground state eigenvector)**.** *Show that if $\psi_0$ is a ground state with $(\psi_0, H\psi_0) = \lambda$ then $H\psi_0 = \lambda\psi_0$, i.e., $\psi_0$ is an eigenvector of $H$ with eigenvalue $\lambda$. (Hint: consider the normalized vector*

$$\phi_\varepsilon = \frac{\psi_0 + \varepsilon\phi}{\|\psi_0 + \varepsilon\phi\|}$$

*for $\phi \in D(H)$. Use that the derivative of $(\phi_\varepsilon, H\phi_\varepsilon)$ wrt. $\varepsilon$ is zero at $\varepsilon = 0$.)*

**PROBLEM 2.6** (Stability of free particle)**.** *Show that the free 1-dimensional particle described in Example 1.8 is stable, but does not have a ground state. Show that its free energy is $F(T) = -\infty$ for all $T > 0$.*

**PROBLEM 2.7** (Gibbs state)**.** *Show that if $\langle\cdot\rangle$ is a Gibbs state at temperature $T > 0$ then*

$$\langle A\rangle = \frac{\mathrm{Tr}(A\exp(-H/T))}{\mathrm{Tr}(\exp(-H/T))}$$

*for all bounded operators $A$. In particular,* $\exp(-H/T)$ *is a trace class operator. (Hint: Use Jensen's inequality and the fact that $t \mapsto t\log t$ is strictly convex. The problem is easier if one assumes that* $\exp(-H/T)$ *is trace class, otherwise some version of the spectral Theorem is needed[4]. )*

Correction since April 15: footnote added

The Hamiltonian $H$ for hydrogen, given in (2) and (3), is stable. It does not have a ground state on the domain $C_0^2$, but in this case, however, this is simply

Correction since April 15: $\infty \to 2$

[3]More generally, a state may be defined as a normalized positive linear functional on the bounded operators on $\mathcal{H}$ (or even on some other algebra of operators). Here we shall only consider states of the form (9) (see also Problem A.2.2).

[4]Theorem 4.12 is sufficient

because the domain is too small (see Section 5). On the extended domain $H^2(\mathbb{R}^3)$ the Hamiltonian does have a ground state. Finding the correct domain on which a Hamiltonian has a possible ground state is an important issue in quantum mechanics.

In Section 3 we discuss in some generality operators and quadratic forms. We shall only be concerned with the eigenvalues of the operators and not with the continuous part of the spectrum. We therefore do not need to understand the Spectral Theorem in its full generality and we shall not discuss it here. We therefore do not need to understand the more complex questions concerning self-adjointness. We mainly consider semi bounded operators and the corresponding quadratic forms.

The notion of quadratic forms is very essential in quantum mechanics. As we have seen the measurable quantities corresponding to an observable, represented by an operator $A$ are the expectation values which are of the form $(\psi, A\psi)$. In applications to quantum mechanics it is therefore relevant to try to build the general theory as much as possible on knowledge of these expectation values. The map $\psi \mapsto (\psi, A\psi)$ is a special case of a quadratic form.

## 2.1 Many body quantum mechanics

Consider $N$ quantum mechanical particles described on Hilbert spaces $\mathfrak{h}_1, \ldots, \mathfrak{h}_N$ and with Hamilton operators $h_1, \ldots, h_N$. The combined system of these particles is described on the tensor product

$$\mathcal{H}_N = \mathfrak{h}_1 \otimes \cdots \otimes \mathfrak{h}_N.$$

We may identify the operators $h_1, \ldots, h_N$ with operators on this tensor product space. I.e., we identify $h_1, \ldots, h_N$ with the operators

$$h_1 \otimes I \otimes \cdots \otimes I, \quad I \otimes h_2 \otimes I \otimes \cdots \otimes I, \quad \ldots \quad I \otimes I \otimes \cdots \otimes h_N.$$

If the particles are *non-interacting* the Hamiltonian operator for the combined system is simply

$$H_N^{\mathrm{in}} = h_1 + \ldots + h_N.$$

This operator may be defined on the domain

$$D(H_N^{\mathrm{in}}) = \mathrm{span}\{\phi_1 \otimes \cdots \otimes \phi_N \mid \phi_1 \in D(h_1), \ldots, \phi_N \in D(h_N)\}.$$

**PROBLEM 2.8.** *Show that if $D(h_1),\ldots,D(h_N)$ are dense in $\mathfrak{h}_1,\ldots,\mathfrak{h}_N$ respectively then $D(H_N^{\rm in})$ is dense in $\mathcal{H}_N$.*

Correction since April 15: one "if" removed $1 \to N$

**THEOREM 2.9** (ground state of non-interacting particles)**.** *If*

$$e_j = \inf_{\phi\in D(h_j),\|\phi\|=1}(\phi, h_j\phi), \quad j = 1,\ldots,N$$

*are ground state energies of the Hamiltonians $h_1,\ldots,h_N$ then the ground state energy of $H_N^{\rm in}$ is $\sum_{j=1}^N e_j$. Moreover, if $\phi_1,\ldots,\phi_N$ are ground state eigenvectors of $h_1,\ldots,h_N$ then $\phi_1\otimes\cdots\otimes\phi_N$ is a ground state eigenvector for $H_N^{\rm in}$.*

Correction since April 15: $\mathcal{H} \to H$

Correction since August 30, 09: $H_N \to H_N^{\rm in}$

*Proof.* If $\Psi \in D(H_N^{\rm in})$ is a unit vector we may write

$$\Psi = \psi_1\otimes\Psi_1 + \ldots + \psi_K\otimes\Psi_K$$

where $\psi_1,\ldots,\psi_K \in D(h_1)$ and $\Psi_1,\ldots,\Psi_K \in \mathfrak{h}_2\otimes\cdots\otimes\mathfrak{h}_N$ are orthonormal. Since $\Psi$ is a unit vector we have $\|\psi_1\|^2+\ldots+\|\psi_K\|^2 = 1$.

Correction since May 3: $N \to K$

We have

$$(\Psi, h_1\Psi) = \sum_{i=1}^K(\psi_i, h_1\psi_i) \geq \sum_{i=1}^K \|\psi_i\|^2 e_1 = e_1.$$

Hence $(\Psi, H_N^{\rm in}\Psi) \geq \sum_{j=1}^N e_j$.

On the other hand if we, given $\varepsilon > 0$, choose unit vectors $\phi_j \in D(h_j)$, $j = 1,\ldots,N$ such that $(\phi_j, h_j\phi_j) < e_j+\varepsilon$ for $j = 1,\ldots,N$ and define $\Psi = \phi_1\otimes\cdots\otimes\phi_N$. We find that $\Psi$ is a unit vector and

$$(\Psi, H_N^{\rm in}\Psi) = \sum_{j=1}^N(\phi_j, h_j\phi_j) \leq \sum_{j=1}^N e_j + N\varepsilon.$$

It is clear that if $\phi_1,\ldots,\phi_N$ are ground state eigenvectors for $h_1,\ldots,h_N$ then $\Psi$ is a ground state eigenvector for $H_N^{\rm in}$. $\square$

The physically more interesting situation is for *interacting particles*. The most common type of interactions is for two particles to interact pairwise. We talk about 2-body interactions. The interaction of particle $i$ and particle $j$ ($i < j$ say) is described by an operator $W_{ij}$ acting in the Hilbert space $\mathfrak{h}_i\otimes\mathfrak{h}_j$. As we shall now explain we may again identify such an operator with an operator on

$\mathfrak{h}_1 \otimes \cdots \otimes \mathfrak{h}_N$, which we also denote by $W_{ij}$. Let us for simplicity of notation assume that $i = 1$ and $j = 2$. We then identify $W_{12}$ with the operator

Correction since May 3: "by" inserted

$$W_{12} \otimes I \otimes \cdots \otimes I$$

(the number of identity operators in this tensor product is $N - 2$) thinking of $\mathfrak{h}_1 \otimes \cdots \otimes \mathfrak{h}_N = (\mathfrak{h}_1 \otimes \mathfrak{h}_2) \otimes \cdots \otimes \mathfrak{h}_N$.

The interacting Hamiltonian is then formally

$$H_N = H_N^{\text{in}} + \sum_{1 \le i < j \le N} W_{ij} = \sum_{j=1}^{N} h_j + \sum_{1 \le i < j \le N} W_{ij}.$$

The reason this is only formal is that the domain of the operator has to be specified and it may depend on the specific situation.

Determining the ground state energy and possible ground state eigenfunctions of an interacting many particle quantum Hamiltonian is a very difficult problem. It can usually not be done exactly and different approximative methods have been developed and we shall discuss these later.

Finally, we must discuss one of the most important issues of many body quantum mechanics. The question of statistics of identical particles. Assume that the $N$ particles discussed above are identical, i.e.,

$$\mathfrak{h}_1 = \ldots = \mathfrak{h}_N = \mathfrak{h}, \quad h_1 = \ldots = h_N = h.$$

If the particles are interacting we also have that the 2-body potential $W_{ij}$ is the same operator $W$ for all $i$ and $j$ and that $\mathrm{Ex} W \mathrm{Ex} = W$, where Ex is the unitary exchange operator.

When we identify the 1-body Hamiltonian $h$ and the 2-body potential $W$ with operators on $\mathfrak{h} \otimes \cdots \otimes \mathfrak{h}$ we must still write subscripts on them: $h_j$ and $W_{ij}$. This is to indicate on which of the tensor factors they act, e.g.

$$h_1 = h \otimes I \otimes \cdots \otimes I, \quad W_{12} = W \otimes I \otimes \cdots \otimes I.$$

It is now clear that the non-interacting operator $H_N^{\text{in}}$ maps vectors in the subspaces $\bigotimes_{\text{sym}}^N \mathfrak{h}$ and $\bigwedge^N \mathfrak{h}$ into the same subspaces. The operator may therefore be restricted to the domains

$$P_+ D(H_N^{\text{in}}) \quad \text{or} \quad P_- D(H_N^{\text{in}}).$$

If we restrict to the symmetric subspace $\bigotimes_{\rm sym}^N \mathfrak{h}$ we refer to the particles as *bosons* and say that they obey Bose-Einstein statistics. If we restrict to the antisymmetric subspace $\bigwedge^N \mathfrak{h}$ we refer to the particles as *fermions* and say that they obey Fermi-Dirac statistics. As we shall see the physics is very different for these two types of systems.

The interaction Hamiltonian will also formally map the subspaces $\bigotimes_{\rm sym}^N \mathfrak{h}$ and $\bigwedge^N \mathfrak{h}$ into themselves. This is only formal since we have not specified the domain of the interaction Hamiltonian.

We have an immediate corollary to Theorem 2.9.

**COROLLARY 2.10** (Ground state of Bose system). *We consider the Hamiltonian $H_N^{\rm in}$ for $N$ identical particles restricted to the symmetric subspace $\bigotimes_{\rm sym}^N \mathfrak{h}$, i.e., with domain*

$$D_{\rm sym}(H_N^{\rm in}) = P_+ D(H_N^{\rm in}).$$

*The ground state energy of this bosonic system is $Ne$ if $e$ is the ground state energy of $h$. Moreover, if $h$ has a ground state eigenvector $\phi$ then $H_N^{\rm in}$ has the ground state eigenvector $\phi\otimes\cdots\otimes\phi$.*

Note in particular that the ground state energy of $H_N^{\rm in}$ on the symmetric subspace $\bigotimes_{\rm sym}^N \mathfrak{h}$ is the same as on the full Hilbert space $\bigotimes^N \mathfrak{h}$.

The situation for fermions is more complicated and we will return to it later.

*EXAMPLE* 2.11 (Atomic Hamiltonian). The Hamilton operator for $N$ electrons in an atom with nuclear charge $Z$ and with the nucleus situated at the origin is

$$\sum_{i=1}^N(-\tfrac{1}{2}\Delta_i - \frac{Z}{|x_i|}) + \sum_{1\leq i<j\leq N}\frac{1}{|x_i-x_j|}.$$

Since physical electrons are fermions this Hamiltonian should be considered on the antisymmetric Hilbert space $\bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$. We shall return to showing that an atom is stable.

# 3 Semi-bounded operators and quadratic forms

**DEFINITION 3.1** (Positive Operators). An operator $A$ defined on a subspace $D(A)$ of $\mathcal{H}$ is said to be positive (or positive definite) if $(\psi, A\psi) > 0$ for all non-zero $\psi \in D(A)$. It is said to be positive semi-definite if $(\psi, A\psi) \geq 0$ for all $\psi \in D(A)$. In particular, such operators are symmetric.

The notion of positivity induces a partial ordering among operators.

**DEFINITION 3.2** (Operator ordering)**.** If $A$ and $B$ are two operators with $D(A) = D(B)$[5] then we say that $A$ is (strictly) less than $B$ and write $A < B$ if the operator $B - A$ (which is defined on $D(B - A) = D(A) = D(B)$ is a positive definite operator. We write $A \leq B$ if $B - A$ is positive semi-definite.

Correction since April 15: footnote added

**DEFINITION 3.3** (Semi bounded operators)**.** An operator $A$ is said to be bounded below if $A \geq -cI$ for some scalar $c$. Here $I$ denotes the identity operator on $\mathcal{H}$. Likewise an operator $A$ is said to be bounded above if $A \leq cI$.

**DEFINITION 3.4** (Quadratic forms)**.** A quadratic form $Q$ is a mapping $Q : D(Q)\times D(Q) \to \mathbb{C}$ (where $D(Q)$ is a (dense) subspace of $\mathcal{H}$), which is sesquilinear (conjugate linear in the first variable and linear in the second):

$$\begin{aligned} Q(\alpha_1\phi_1 + \alpha_2\phi_2, \psi) &= \overline{\alpha_1}Q(\phi_1, \psi) + \overline{\alpha_2}Q(\phi_2, \psi) \\ Q(\phi, \alpha_1\psi_1 + \alpha_2\psi_2) &= \alpha_1 Q(\phi, \psi_1) + \alpha_2 Q(\phi, \psi_2). \end{aligned}$$

We shall often make a slight abuse of notation and denote $Q(\phi, \phi)$ by $Q(\phi)$. A quadratic form $Q$ is said to be positive definite if $Q(\phi) > 0$ for all $\phi \neq 0$ and positive semi-definite if $Q(\phi) \geq 0$. It is said to be bounded below if $Q(\phi) \geq -c\|\phi\|^2$ (and above if $Q(\phi) \leq c\|\phi\|^2$) for some $c \in \mathbb{R}$.

**PROBLEM 3.5** (Cauchy-Schwarz inequality)**.** *Show that if $Q$ is a positive semi-definite quadratic form it satisfies the Cauchy-Schwarz inequality*

$$|Q(\phi, \psi)| \leq Q(\phi)^{1/2}Q(\psi)^{1/2}. \tag{10}$$

**DEFINITION 3.6** (Bounded quadratic forms)**.** A quadratic form $Q$ is said to be bounded if there exists $0 \leq M < \infty$ such that

$$|Q(\phi)| \leq M\|\phi\|^2,$$

for all $\phi \in D(Q)$.

[5] It would be more correct to say that we require that $D(A) \cap D(B)$ is dense and that $B - A$ is positive (semi)-definite on this subspace

Note that quadratic forms that are bounded above and below are bounded, but the converse is not true since bounded quadratic forms are not necessarily real.

As for operators we have that if $Q$ is positive semi-definite (or even just bounded above or below) then it is symmetric, meaning

$$Q(\phi,\psi) = \overline{Q(\psi,\phi)}. \tag{11}$$

The proof is the same as in Problem 1.6.

**PROBLEM 3.7.** *Show that if $Q$ is a bounded quadratic form then it extends to a unique bounded quadratic form on all of $\mathcal{H}$ (compare Problem 1.10).*

**PROBLEM 3.8.** *Show that if $Q$ is a quadratic form then it is enough to know, $Q(\phi) = Q(\phi,\phi)$ for all $\phi \in D(Q)$, in order to determine $Q(\psi_1,\psi_2)$ for all $\psi_1,\psi_2 \in D(Q)$.*

Correction since April 15: "All" added

It is clear that to an operator $A$ we have a corresponding quadratic form $Q(\phi) = (\phi, A\phi)$. The next problem shows that the opposite is also true.

**PROBLEM 3.9** (Operators corresponding to quadratic forms)**.** *Show that corresponding to a quadratic form there exists a unique linear map $A : D(A) \to \mathcal{H}$, with*

$$D(A) = \left\{ \phi \in D(Q) : \sup_{\psi \in D(Q)\setminus\{0\}} \frac{|Q(\psi,\phi)|}{\|\psi\|} < \infty \right\}$$

*such that $Q(\psi,\phi) = (\psi, A\phi)$ for all $\phi \in D(A)$ and $\psi \in D(Q)$. Note, that we may have that $D(A)$ is a strict subspace of $D(Q)$. In fact, in general $D(A)$ need not even be dense (see Example 5.4).*

Correction since April 15: operator→ linear map. Formulation improved to $Q(\psi,\phi) = (\psi, A\phi)$ for all $\phi \in D(A)$ and $\psi \in D(Q)$

The quadratic form corresponding to a Schrödinger operator $-\frac{1}{2}\Delta + V$ is

$$\begin{aligned} Q(\phi) &= -\tfrac{1}{2}\int \overline{\phi(x)}\Delta\phi(x)dx + \int V(x)|\phi(x)|^2 dx \\ &= \tfrac{1}{2}\int |\nabla\phi(x)|^2 dx + \int V(x)|\phi(x)|^2 dx \end{aligned}$$

for $\phi$ being a $C_0^2$ function. In Section 11.3 in Lieb and Loss Analysis[6] conditions are given on the potential $V$ that ensure that the quadratic form corresponding to a Schrödinger operator can be extended to the Sobolev space $H^1(\mathbb{R}^3)$.

Correction since April 15: $C_0^\infty \to C_0^2$

[6]Lieb and Loss *Analysis*, AMS Graduate Studies in Mathematics Vol. **114** 2nd edition

**PROBLEM 3.10.** *Assume that $Q$ is a quadratic form, which is bounded below and that $A$ is the corresponding operator defined in Problem 3.9. If a unit vector $\psi_0 \in D(Q)$ satisfies that*

$$Q(\psi_0) = \inf_{\phi\in D(Q),\|\phi\|=1} Q(\phi)$$

*show that $\psi_0$ is a ground state eigenvector for $A$.*

*Theorem 11.5 in Lieb and Loss Analysis gives conditions ensuring that a Schrödinger operator has a ground state.*

# 4 Extensions of operators and quadratic forms

We shall here briefly sketch how to define a natural extension of a symmetric operator and how to define a natural extension of the corresponding quadratic form if the operator is bounded below.

**DEFINITION 4.1** (Closed operator)**.** An operator $A$ on a Hilbert space $\mathcal{H}$ is said to be closed if its *graph*

Correction since April 15: $\in \mathcal{H}\oplus\mathcal{H}$ added

$$\mathcal{G}(A) = \{(\phi, A\phi) \in \mathcal{H}\oplus\mathcal{H} \mid \phi \in D(A)\}$$

is closed in the Hilbert space $\mathcal{H}\oplus\mathcal{H}$.

**THEOREM 4.2** (Closability of symmetric operator)**.** *If $A$ is a symmetric (densely defined) operator on a Hilbert space $\mathcal{H}$ then the closure of its graph $\overline{\mathcal{G}(A)}$ is the graph of a closed operator $\overline{A}$, the closure of $A$.*

*Proof.* We have to show that we can define an operator $\overline{A}$ with domain

$$D(\overline{A}) = \{\phi \in \mathcal{H} \mid \exists\psi \in \mathcal{H} : (\phi, \psi) \in \overline{\mathcal{G}(A)}\}$$

such that for $\phi \in D(\overline{A})$ we have $\overline{A}\phi = \psi$ if $(\phi, \psi) \in \overline{\mathcal{G}(A)}$. The only difficulty in proving that this defines a closed (linear) operator is to show that there is at most one $\psi$ for which $(\phi, \psi) \in \overline{\mathcal{G}(A)}$. Thus we have to show that if $(0, \psi) \in \overline{\mathcal{G}(A)}$ then $\psi = 0$.

If $(0, \psi) \in \overline{\mathcal{G}(A)}$ we have a sequence $\phi_n \in D(A)$ with $\lim_{n\to\infty} \phi_n = 0$ and $\lim_{n\to\infty} A\phi_n = \psi$. For all $\phi' \in D(A)$ we then have since $A$ is symmetric that

$$(\phi', \psi) = \lim_{n\to\infty} (\phi', A\phi_n) = \lim_{n\to\infty} (A\phi', \phi_n) = 0.$$

Thus $\psi \in D(A)^\perp$, but since $D(A)$ is dense we have $\psi = 0$. $\square$

*EXAMPLE* 4.3. If we consider the Laplace operator with domain $C_0^2(\mathbb{R}^n)$, then the domain of the closure is the Sobolev space $H^2(\mathbb{R}^n)$.

Correction since April 15: $C_0^\infty \to C_0^2$

**DEFINITION 4.4** (Closed quadratic form)**.** A quadratic form $Q$ satisfying the lower bound $Q(\phi) \geq -\alpha\|\phi\|^2$ for some $\alpha > 0$ is said to be closed if the domain $D(Q)$ is complete under the norm

$$\|\phi\|_\alpha = \sqrt{(\alpha+1)\|\phi\|^2 + Q(\phi)}.$$

(That this is a norm follows from the Cauchy-Schwarz inequality in Problem 3.5.)

**PROBLEM 4.5.** *Show that the above definition does not depend on how large $\alpha$ is chosen.*

Correction since April 15: symmetric $\to$ semibounded. $Q(\phi) \geq -\alpha\|\phi\|^2$ added.

**THEOREM 4.6** (Closability of form coming from semibounded operator)**.** *Let $A$ be a (densely defined) operator on a Hilbert space $\mathcal{H}$ with the lower bound $A \geq -\alpha I$ for some $\alpha > 0$. Then there exists a unique closed quadratic form $Q$ such that*

- *$D(A) \subseteq D(Q)$.*
- *$D(Q)$ is the closure of $D(A)$ under the norm $\|\cdot\|_\alpha$.*
- *$Q(\phi) \geq -\alpha\|\phi\|^2$*
- *$Q(\phi) = (\phi, A\phi)$ for $\phi \in D(A)$.*

*Proof.* We consider the norm

$$\|\phi\|_\alpha = \sqrt{(\alpha+1)\|\phi\|^2 + (\phi, A\phi)}$$

defined for $\phi \in D(A)$. Observe that $\|\phi\| \leq \|\phi\|_\alpha$. Thus if $\phi_n \in D(A)$ is a Cauchy sequence for the norm $\|\cdot\|_\alpha$ it is also a Cauchy sequence for the original norm $\|\cdot\|$. Hence there is a $\phi \in \mathcal{H}$ such that $\lim_{n\to\infty} \phi_n = \phi$. Moreover, since $\|\cdot\|_\alpha$ is a norm it follows that $\|\phi_n\|_\alpha$ is a Cauchy sequence of real numbers, which hence converges to a real number. Since $\lim_{n\to\infty}\|\phi_n\| = \|\phi\|$ we conclude that the sequence $(\phi_n, A\phi_n)$ converges to a real number.

We want to define the quadratic form $Q$ having domain $D(Q)$ consisting of all vectors $\phi \in \mathcal{H}$ for which there is a Cauchy sequence $\phi_n \in D(A)$ under the $\|\cdot\|_\alpha$ norm such that $\lim_{n\to\infty}\phi_n = \phi$. For such a $\phi$ we define $Q(\phi) = \lim_{n\to\infty}(\phi_n, A\phi_n)$. The only difficulty in proving the theorem is to show that $\phi = 0$ implies that $\lim_{n\to\infty}(\phi_n, A\phi_n) = 0$. In fact, all we have to show is that $\lim_{n\to\infty}\|\phi_n\|_\alpha = 0$. Let us denote by

$$(\psi', \psi)_\alpha = (\alpha+1)(\psi', \psi) + (\psi', A\psi)$$

the inner product corresponding to the norm $\|\cdot\|_\alpha$. Then

$$\|\phi_n\|_\alpha^2 = (\phi_n, \phi_m)_\alpha + (\phi_n, \phi_n - \phi_m)_\alpha \leq |(\phi_n, \phi_m)_\alpha| + \|\phi_n\|_\alpha \|\phi_n - \phi_m\|_\alpha.$$

The second term tends to zero as $n$ tends to infinity with $m \geq n$ since $\phi_n$ is a Cauchy sequence for the $\|\cdot\|_\alpha$ norm and $\|\phi_n\|_\alpha$ is bounded. For the first term above we have since $A$ is symmetric

Correction since April 15: absolute values inserted

$$(\phi_n, \phi_m)_\alpha = (\alpha+1)(\phi_n, \phi_m) + (\phi_n, A\phi_m) = (\alpha+1)(\phi_n, \phi_m) + (A\phi_n, \phi_m).$$

This tends to 0 as $m$ tends to infinity since $\lim_{m\to\infty}\phi_m = \phi = 0$. □

*EXAMPLE* 4.7. If we consider the Laplace operator with domain $C_0^2(\mathbb{R}^n)$, then the domain of the closed quadratic form in the theorem above is the Sobolev space $H^1(\mathbb{R}^n)$.

Correction since April 15: $C_0^\infty \to C_0^2$

**DEFINITION 4.8** (Friedrichs' extension)**.** The symmetric operator which according to Problem 3.9 corresponds to the closed quadratic form $Q$ described in Theorem 4.6 is called the *Friedrichs' extension* of the operator $A$, we will denote it $A_{\mathrm{F}}$.

Correction since April 15: Notation $A_{\mathrm{F}}$ added

We will in the future often prove results on conveniently chosen domains. These results may then by continuity be extended to the naturally extended domain for the Friedrichs' extension.

In particular we see that stable Hamiltonians $H$ have a Friedrichs' extension.

**PROBLEM 4.9.** *Show that the Friedrichs' extension of an operator is a closed operator and hence that* $\overline{A} \subseteq A_{\mathrm{F}}$.

**PROBLEM 4.10.** *Argue that Friedrichs extending an operator that is already a Friedrichs extension does not change the operator, i.e.,* $(A_{\mathrm{F}})_{\mathrm{F}} = A_{\mathrm{F}}$.

Hence the Friedrichs extension is in general a larger extension than the closure of the operator. In Problem 5.19 we shall see that the Friedrichs extension may in fact be strictly larger than the closure.

**PROBLEM 4.11.** *Show that if $A$ is bounded below then the Friedrichs' extension of $A+\lambda I$ (defined on $D(A)$) for some $\lambda \in \mathbb{R}$ is $(A+\lambda I)_{\mathrm{F}} = A_F + \lambda I$ defined on $D(A_F)$.*

We have seen that symmetric operators are characterized by $A \subseteq A^*$. The Friedrichs' extensions belong to the more restrictive class of *self-adjoint operators* satisfying $A = A^*$ [7] . Self-adjoint operators are very important. It is for this class of operators that one has a general spectral theorem. We will here not discuss selfadjoint operators in general, but restrict attention to Friedrichs' extensions. The closure of a symmetric operator is in general not self-adjoint. If it is the operator is called *essentially self-adjoint.*

Correction since August 30, 09: footnote added

Short of giving the full spectral theorem we will in the next theorem characterize the part of the spectrum of a Friedrichs' extension which corresponds to eigenvalues below the *essential spectrum.* We will not here discuss the essential spectrum, it includes the continuous spectrum but also eigenvalues of infinite multiplicity.

In these lecture notes we will only be interested in aspects of physical systems which may be understood solely from the eigenvalues below the essential spectrum. For hydrogen the spectrum is the set

$$\left\{ -\frac{1}{2n^2} \ : \ n = 1, 2, \ldots \right\} \cup [0, \infty).$$

The essential spectrum $[0,\infty)$ corresponds here to the continuous spectrum. The eigenvalues can be characterize as in the theorem below. In the next section we will do this for the ground state energy.

**THEOREM 4.12** (Min-max principle for Friedrichs' extension)**.** *Consider an operator $A$ which is bounded from below on a Hilbert space $\mathcal{H}$. Define the sequence*

$$\mu_n = \mu_n(A) = \inf \left\{ \max_{\phi \in M, \ \|\phi\|=1} (\phi, A\phi) \ : \ M \subseteq D(A), \quad \dim M = n \right\}. \tag{12}$$

[7] see Appendix A.4.1

*Then $\mu_n$ is a non-decreasing sequence and unless $\mu_1, \ldots, \mu_k$ are eigenvalues of the Friedrichs' extension $A_{\mathrm{F}}$ of $A$ counted with multiplicities we have*

$$\mu_k = \mu_{k+1} = \mu_{k+2} = \ldots .$$

*If this holds we call $\mu_k$ the bottom of the essential spectrum.*

Correction since August 30, 09: $\mu_{k=2} \to \mu_{k+2}$

*If $\mu_k < \mu_{k+1}$ then the infimum above for $n = k$ is attained for the $k$-dimensional space $M_k$ spanned by the eigenfunctions of $A_{\mathrm{F}}$ corresponding to the eigenvalues $\mu_1, \ldots, \mu_k$ in the sense that*

Correction since May 3: Formulation changed slightly

$$\mu_k = \max_{\phi \in M_k,\ \|\phi\|=1} (\phi, A_{\mathrm{F}}\phi),$$

*If $\phi \in M_k^{\perp} \cap D(A_{\mathrm{F}})$ then $(\phi, A_{\mathrm{F}}\phi) \geq \mu_{k+1}\|\phi\|^2$.*

*On the other hand if $\mu_1, \ldots, \mu_k$ are eigenvalues for $A_{\mathrm{F}}$ with corresponding eigenvectors spanning a $k$-dimensional space $M_k$ such that $(\phi, A_{\mathrm{F}}\phi) \geq \mu_k\|\phi\|^2$ for all $\phi \in M_k^{\perp} \cap D(Q)$ then (12) holds for $n = 1, \ldots, k$.*

The proof is given in Appendix C. Note in particular that since $A$ is assumed to be bounded from below

$$\mu_1(A) = \inf_{\phi \in D(A),\ \|\phi\|=1} (\phi, A\phi) > -\infty. \tag{13}$$

**PROBLEM 4.13.** *Show that if $\mu_n$ are the min-max values defined in Theorem 4.12 for an operator $A$ which is bounded below then*

$$\sum_{n=1}^{N} \mu_n(A) =$$
$$\inf\{\mathrm{Tr}(PA) \mid P \text{ an orth. proj. onto an } N\text{-dimensional subspace of } D(A)\}.$$

**PROBLEM 4.14** (Operators with compact resolvent)**.** *Assume that the min-max values $\mu_n(A)$ of an operator $A$ on a Hilbert space $\mathcal{H}$ which is bounded below satisfy $\mu_n(A) \to \infty$ as $n \to \infty$. Show that we may choose an orthonormal basis of $\mathcal{H}$ consisting of eigenvectors of $A_{\mathrm{F}}$.*

*Show that there is a constant $\alpha > 0$ such that the Friedrichs' extension of $A + \alpha I$ (defined on $D(A)$) is an injective operator that maps onto all of the Hilbert space. Show that the inverse map $(A_F + \alpha I)^{-1}$ is compact. The operator $(A_F + \alpha I)^{-1}$ is called a resolvent of $A$ and we say that $A$ has compact resolvent.*

Correction since August 30, 09: $A \to A_F$

# 5 Schrödinger operators

We shall in this section discuss Schrödinger operators (see Example 1.15) in more details.

**DEFINITION 5.1** (Schrödinger operator on $C_0^2(\mathbb{R}^n)$)**.** The Schrödinger operator for a particle without internal degrees of freedom moving in a potential $V \in L^2_{\text{loc}}(\mathbb{R}^n)^8$

$$H = -\tfrac{1}{2}\Delta - V$$

with domain $D(H) = C_0^2(\mathbb{R}^n)$.

As we saw earlier we also have the Schrödinger quadratic form.

**DEFINITION 5.2** (Schrödinger quadratic form on $C_0^1(\mathbb{R}^n)$)**.** The Schrödinger quadratic form for a particle without internal degrees of freedom moving in a potential $V \in L^1_{\text{loc}}(\mathbb{R}^n)$ is

$$Q(\phi) = \tfrac{1}{2}\int_{\mathbb{R}^n} |\nabla\phi|^2 - \int_{\mathbb{R}^n} V|\phi|^2$$

with domain $D(Q) = C_0^1(\mathbb{R}^n)$.

Note that in order to define the quadratic form on $C_0^1(\mathbb{R}^n)$ we need only assume that $V \in L^1_{\text{loc}}$ whereas for the operator we need $V \in L^2_{\text{loc}}$.

**PROBLEM 5.3.** *If $V \in L^2_{\text{loc}}$ show that the operator defined as explained in Problem 3.9 from the Schrödinger quadratic form $Q$ with $D(Q) = C_0^1(\mathbb{R}^n)$ is indeed an extension of the Schrödinger operator $H = -\Delta - V$ to a domain which includes $C_0^2(\mathbb{R}^n)$. If $V \in L^1_{\text{loc}} \setminus L^2_{\text{loc}}$ then this need not be the case as explained in the next example.*

*EXAMPLE* 5.4. Consider the function $f : \mathbb{R}^n \to \mathbb{R}$ given by

$$f(x) = \begin{cases} |x|^{-n/2}, & \text{if } |x| < 1 \\ 0, & \text{otherwise} \end{cases}$$

Then $f$ is in $L^1(\mathbb{R}^n)$ but not in $L^2(\mathbb{R}^n)$. Let $q_1, q_2, \ldots$ be an enumeration of the rational points in $\mathbb{R}^n$ and define $V(x) = \sum_i i^{-2} f(x - q_i)$. Then $V \in L^1(\mathbb{R}^n)$ but for all $\psi \in C_0^1(\mathbb{R}^n)\backslash 0$ we have $V\psi \notin L^2$. This follows easily since $|V(x)|^2|\psi(x)|^2 \geq i^{-2}|x-q_i|^{-n}|\psi(x)|^2$ for all $i$. Therefore the domain of the operator $A$ defined from the Schrödinger quadratic form $Q$ with $D(Q) = C_0^1(\mathbb{R}^n)$ is $D(A) = \{0\}$.

Correction since August 30, 09: $V \in L^1_{\mathrm{loc}} \to V \in L^1$; $C_0^1(\mathbb{R}^n) \to C_0^1(\mathbb{R}^n)\backslash\{0\}$

We shall now discuss ways of proving that the Schrödinger quadratic form is bounded from below.

We begin with the Perron-Frobenius Theorem for the Schrödinger operator. Namely, the fact that if we have found a non-negative eigenfunction for the Schrödinger operator then the corresponding eigenvalue is the lowest possible expectation for the Schrödinger quadratic form.

**THEOREM 5.5** (Perron-Frobenius for Schrödinger). *Let $V \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$. Assume that $0 < \psi \in C^2(\Omega)$ and that $(-\frac{1}{2}\Delta - V)\psi(x) = \lambda\psi(x)$ for all $x$ in some open set $\Omega$. Then for all $\phi \in C_0^1(\mathbb{R}^n)$ with support in $\Omega$ we have*

$$Q(\phi) = \tfrac{1}{2}\int_{\mathbb{R}^n} |\nabla\phi|^2 - \int_{\mathbb{R}^n} V|\phi|^2 \geq \lambda \int_{\mathbb{R}^n} |\phi|^2.$$

Correction since August 30, 09: $C^2(\mathbb{R}^n) \cap L^2(\mathbb{R}^n) \to C^2(\Omega)$. In the Corollary below $\psi(x) = e^{-Z|x|} \notin C^1(\mathbb{R}^N)$.

*Proof.* Given $\phi \in C_0^1(\mathbb{R}^n)$ we can write $\phi = f\psi$, where $f \in C_0^1(\mathbb{R}^n)$. Then

$$\begin{aligned} Q(\phi) &= \tfrac{1}{2}\int_{\mathbb{R}^n} \left[\psi^2|\nabla f|^2 + |f|^2|\nabla\psi|^2 + \left(\overline{f}\nabla f + f\overline{\nabla f}\right)\psi\nabla\psi\right] - \int_{\mathbb{R}^n} V|f\psi|^2 \\ &\geq \tfrac{1}{2}\int_{\mathbb{R}^n} \left[|f|^2|\nabla\psi|^2 + \left(\overline{f}\nabla f + f\overline{\nabla f}\right)\psi\nabla\psi\right] - \int_{\mathbb{R}^n} V|f\psi|^2 \\ &= \int_{\mathbb{R}^n} \left[|f|^2\psi(-\tfrac{1}{2}\Delta - V)\psi\right] = \lambda\int_{\mathbb{R}^n} |\phi|^2, \end{aligned}$$

where the second to last identity follows by integration by parts. $\square$

**COROLLARY 5.6** (Lower bound on hydrogen). *For all $\phi \in C_0^1(\mathbb{R}^3)$ we have*

$$\tfrac{1}{2}\int |\nabla\phi(x)|^2 dx - \int Z|x|^{-1}|\phi(x)|^2 dx \geq -\frac{Z^2}{2}\int |\phi(x)|^2 dx.$$

*Proof.* Consider the function $\psi(x) = e^{-Z|x|}$. Then for all $x \neq 0$ we have

$$(-\tfrac{1}{2}\Delta - Z|x|^{-1})\psi(x) = -\frac{Z^2}{2}\psi(x).$$

The statement therefore immediately follows for all $\phi \in C_0^1(\mathbb{R}^3)$ with support away from 0 from the previous theorem. The corollary follows for all $\phi \in C_0^1(\mathbb{R}^3)$ using the result of the next problem. $\square$

[8]The space $L^p_{\mathrm{loc}}(\mathbb{R}^n)$, for some $p \geq 1$ consists of functions $f$ (defined modulo sets of measure zero), such that $\int_{\mathcal{C}} |f|^p < \infty$ for any compact set $\mathcal{C} \subset \mathbb{R}^n$

**PROBLEM 5.7.** *Show that all $\phi \in C_0^1(\mathbb{R}^3)$ can be approximated by functions $\phi_n \in C_0^1(\mathbb{R}^3)$ with support away from 0 in such a way that*

$$\int |\nabla\phi_n(x)|^2 dx - \int Z|x|^{-1}|\phi_n(x)|^2 dx \to \int |\nabla\phi(x)|^2 dx - \int Z|x|^{-1}|\phi(x)|^2 dx.$$

**PROBLEM 5.8.** *Show that the function $\psi(x) = e^{-Z|x|}$ as a function in $L^2(\mathbb{R}^3)$ is an eigenfunction with eigenvalue $-Z^2/2$ for the Friedrichs' extension of $H = -\frac{1}{2}\Delta - Z|x|^{-1}$ (originally) defined on $C_0^2(\mathbb{R}^3)$.*

It is rarely possible to find positive eigenfunctions. A much more general approach to proving lower bounds on Schrödinger quadratic forms is to use the Sobolev inequality. In a certain sense this inequality is an expression of the celebrated uncertainty principle.

**THEOREM 5.9** (Sobolev Inequality)**.** *For all $\phi \in C_0^1(\mathbb{R}^n)$ with $n \geq 3$ we have the Sobolev inequality*

$$\|\phi\|_{\frac{2n}{n-2}} \leq \frac{2(n-1)}{n-2}\|\nabla\phi\|_2$$

*Proof.* Let $u \in C_0^1(\mathbb{R}^n)$ then we have

$$u(x) = \int_{-\infty}^{x_i} \partial_i u(x_1, \ldots, x_{i-1}, x_i', x_{i+1}, \ldots, x_n) dx_i'.$$

Hence

$$|u(x)|^{\frac{n}{n-1}} \leq \left(\prod_{i=1}^n \int_{-\infty}^{\infty} |\partial_i u| dx_i\right)^{\frac{1}{n-1}}.$$

Thus by the general Hölder inequality (in the case $n = 3$ simply by Cauchy-Schwarz)

$$\int_{-\infty}^{\infty} |u(x)|^{\frac{n}{n-1}} dx_1 \leq \left(\int_{-\infty}^{\infty} |\partial_1 u| dx_1\right)^{\frac{1}{n-1}} \left(\prod_{i=2}^n \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\partial_i u| dx_1 dx_i\right)^{\frac{1}{n-1}}.$$

Using the same argument for repeated integrations over $x_2, \ldots, x_n$ gives

$$\int_{\mathbb{R}^n} |u(x)|^{\frac{n}{n-1}} dx \leq \left(\prod_{i=1}^n \int_{\mathbb{R}^n} |\partial_i u| dx\right)^{\frac{1}{n-1}}.$$

Thus

$$\|u\|_{\frac{n}{n-1}} \leq \|\nabla u\|_1.$$

Now set $u = \phi^{\frac{2(n-1)}{n-2}}$. (The reader may at this point worry about the fact that $u$ is not necessarily $C^1$. One can easily convince oneself that the above argument works for this $u$ too. Alternatively , in the case $n = 3$ which is the one of interest here $\frac{2(n-1)}{n-2}$ is an integer and thus $u$ is actually $C^1$.) We then get

$$\|\phi\|_{\frac{2n}{n-2}}^{\frac{2(n-1)}{n-2}} \leq \frac{2(n-1)}{n-2}\|\phi\|_{\frac{2n}{n-2}}^{\frac{n}{n-2}}\|\nabla\phi\|_2.$$

□

Especially for $n = 3$ we get

$$\|\phi\|_6 \leq 4\|\nabla\phi\|_2.$$

The sharp constant in the Sobolev inequality was found by Talenti[9] In the case $n = 3$ the sharp version of the Sobolev inequality is

Correction since August 30, 09: In footnote Vol. 114 → Vol. 14.

$$\|\phi\|_6 \leq \frac{\sqrt{3}}{2}(2\pi^2)^{1/3}\|\nabla\phi\|_2 \approx 2.34\|\nabla\phi\|_2. \tag{14}$$

**THEOREM 5.10** (Sobolev lower bound on Schrödinger)**.** *Assume that* $V \in L^1_{\rm loc}(\mathbb{R}^n)$, $n \geq 3$ *and that the positive part* $V_+ = \max\{V, 0\}$ *of the potential satisfies* $V_+ \in L^{\frac{2+n}{2}}(\mathbb{R}^n)$. *Then for all* $\phi \in C_0^1(\mathbb{R}^n)$ *we get*

$$\begin{aligned} Q(\phi) &= \tfrac{1}{2}\int_{\mathbb{R}^n}|\nabla\phi|^2 - \int_{\mathbb{R}^n} V|\phi|^2 \\ &\geq -\frac{2}{n+2}\left(\frac{2n}{n+2}\right)^{n/2}\left(\frac{2(n-1)}{n-2}\right)^n\left(\int V_+^{\frac{2+n}{2}}\right)\|\phi\|_2^2 \end{aligned}$$

*Proof.* In order to prove a lower bound we may of course replace $V$ by $V_+$. We use the Sobolev Inequality and Hölder's inequality

$$Q(\phi) \geq \frac{1}{2}\left(\frac{2(n-1)}{n-2}\right)^{-2}\|\phi\|^2_{\frac{2n}{n-2}} - \|V_+\|_{\frac{2+n}{2}}\|\phi\|_{\frac{2n}{n-2}}^{\frac{2n}{n+2}}\|\phi\|_2^{\frac{4}{n+2}}.$$

We get a lower bound by minimizing over $t = \|\phi\|^2_{\frac{2n}{n-2}}$, i.e.,

$$Q(\phi) \geq \min_{t\geq 0}\left\{\frac{1}{2}\left(\frac{2(n-1)}{n-2}\right)^{-2} t - \|V_+\|_{\frac{2+n}{2}}\|\phi\|_2^{\frac{4}{n+2}}t^{\frac{n}{n+2}}\right\},$$

which gives the answer above. □

[9] Talenti, G. *Best constant in Sobolev inequality*, Ann. Mat. Pura Appl. **110** (1976), 353–372. See the book *Analysis*, AMS Graduate Studies in Mathematics Vol. **14** by Lieb and Loss for a simple proof.

For $n = 3$ we find

$$Q(\phi) \geq -\frac{768}{25}\sqrt{\frac{6}{5}}\left(\int V_+^{5/2}\right)\|\phi\|_2^2 \approx -33.65\left(\int V_+^{5/2}\right)\|\phi\|_2^2.$$

**PROBLEM 5.11.** *Show that using the sharp Sobolev inequality (14) we get*

$$Q(\phi) \geq -\frac{27\pi^2}{25}\sqrt{\frac{2}{5}}\left(\int V_+^{5/2}\right)\|\phi\|_2^2 \approx -6.74\left(\int V_+^{5/2}\right)\|\phi\|_2^2. \tag{15}$$

**PROBLEM 5.12** (Positivity of Schrödinger quadratic form)**.** *Show that if $V_+ \in L^{3/2}(\mathbb{R}^3)$ and if the norm $\|V_+\|_{3/2}$ is small enough then*

$$Q(\phi) = \frac{1}{2}\int_{\mathbb{R}^3}|\nabla\phi|^2 - \int_{\mathbb{R}^3} V|\phi|^2 \geq 0$$

*for all $\phi \in C_0^1(\mathbb{R}^3)$.*

**PROBLEM 5.13.** *Show that if $n \geq 3$ and $V = V_1 + V_2$, where $V_1 \in L^\infty(\mathbb{R}^n)$ and $V_2 \in L^{n/2}(\mathbb{R}^n)$ with $\|V_2\|_{n/2}$ small enough then the closed quadratic form defined in Theorem 4.6 corresponding to the operator $-\frac{1}{2}\Delta - V$ defined originally on $C_0^2(\mathbb{R}^n)$ has domain $H^1(\mathbb{R}^n)$. [Hint: You may use that $H^1(\mathbb{R}^n)$ is the domain of the closed quadratic form in the case $V = 0$]* Correction since May 3: $3 \to n$

*EXAMPLE* 5.14 (Sobolev lower bound on hydrogen)*.* We now use the Sobolev inequality to give a lower bound on the hydrogen quadratic form

$$Q(\phi) = \frac{1}{2}\int_{\mathbb{R}^3}|\nabla\phi|^2 - \int_{\mathbb{R}^3} Z|x|^{-1}|\phi|^2.$$

In Corollary 5.6 we of course already found the sharp lower bound for the hydrogen energy. This example serves more as a test of the applicability of the Sobolev inequality.

For all $R > 0$

$$Q(\phi) \geq \frac{1}{2}\int_{\mathbb{R}^3}|\nabla\phi|^2 - \int_{|x|\leq R} Z|x|^{-1}|\phi|^2 - ZR^{-1}\int_{\mathbb{R}^3}|\phi|^2.$$

Using (15) we find

$$\begin{aligned} Q(\phi) &\geq \left[-\frac{27\pi^2}{25}\sqrt{\frac{2}{5}}\left(\int_{|x|<R} Z^{5/2}|x|^{-5/2}\right) - ZR^{-1}\right]\int_{\mathbb{R}^3}|\phi|^2 \\ &\approx -169.43Z^{5/2}R^{1/2} - ZR^{-1} \geq -57.87Z^2, \end{aligned}$$

where we have minimized over $R$. This result should be compared with the sharp value $-0.5Z^2$.

We may think of the Sobolev lower bound Theorem 5.10 as a bound on the first min-max value $\mu_1$ (independetly of whether it is an eigenvalue or not) of $-\frac{1}{2}\Delta - V(x)$. The Sobolev bound may be strengthened to the following result. A proof may be found in Lieb and Loss, Analysis, Theorem 12.4.

**THEOREM 5.15** (Lieb-Thirring inequality)**.** *There exists a constant $C_{\rm LT} > 0$ such that if $V \in L^2_{\rm loc}(\mathbb{R}^n)$ and $V_+ \in L^{(n+2)/2}(\mathbb{R}^n)$ then the min-max values $\mu_n$ for $-\frac{1}{2}\Delta - V(x)$ defined on $C_0^2(\mathbb{R}^n)$ satisfy*

$$\sum_{n=1}^{\infty} \mu_n \geq -C_{\rm LT} \int V_+^{(n+2)/2}.$$

Correction since August 30, 09: $\sum_{n=0}^{\infty} \mu_n \to \sum_{n=1}^{\infty} \mu_n$.

**PROBLEM 5.16** (Hardy's Inequality)**.** *Show that for all $\phi \in C_0^1(\mathbb{R}^3)$ we have*

$$\int_{\mathbb{R}^3} |\nabla \phi(x)|^2 dx \geq \frac{1}{4} \int_{\mathbb{R}^3} |x|^{-2} |\phi(x)|^2 dx.$$

*Show also that $1/4$ is the sharp constant in this inequality.*

*EXAMPLE* 5.17 (Dirichlet and Neumann Boundary conditions). Consider the quadratic form

$$Q(\phi) = \int_0^1 |\phi'|^2$$

on the Hilbert space $L^2([0,1])$ with the domain

$$D_0(Q) = \left\{ \phi \in C^1([0,1]) : \phi(0) = \phi(1) = 0 \right\}$$

or

$$D_1(Q) = C^1([0,1]).$$

The operator $A_0$ corresponding to $Q$ according to Problem 3.9 with domain $D_0(Q)$ satisfies that

Correction since May 3: $= D(A_0) \cap C^2([0,1])$ added

$$\left\{ \phi \in C^2([0,1]) : \phi(0) = \phi(1) = 0 \right\} = D(A_0) \cap C^2([0,1])$$

and if $\phi \in C^2([0,1])$ with $\phi(0) = \phi(1) = 0$ then $A_0 \phi = -\phi''$. This follows by integration by parts since if $\psi \in D_0(Q)$ then

$$Q(\psi, \phi) = \int_0^1 \overline{\psi'} \phi' = \phi'(1)\overline{\psi(1)} - \phi'(0)\overline{\psi(0)} - \int_0^1 \overline{\psi} \phi'' = -\int \overline{\psi} \phi''.$$

The condition $\phi(0) = \phi(1) = 0$ is called the *Dirichlet boundary condition*.

The operator $A_1$ corresponding to $Q$ with domain $D_1(Q)$ satisfies that

Correction since May 3: $= D(A_1) \cap C^2([0,1])$ added

$$\{\phi \in C^2([0,1]) : \phi'(0) = \phi'(1) = 0\} = D(A_1) \cap C^2([0,1])$$

and if $\phi \in C^2([0,1])$ with $\phi'(0) = \phi'(1) = 0$ then $A_1\phi = -\phi''$. Note that this time there was no boundary condition in the domain $D_1(Q)$, but it appeared in the domain of $A_1$. The boundary condition $\phi'(0) = \phi'(1) = 0$ is called the *Neumann boundary condition*. The statement again follows by integration by parts as above. This time the boundary terms do not vanish automatically. Since the map $(\psi, \phi) \mapsto \phi'(1)\overline{\psi(1)}$ is not bounded on $L^2$ we have to ensure the vanishing of the boundary terms in the definition of the domain of $A_1$.

The operators $A_1$ and $A_0$ are both extensions of the operator $A = -\frac{d^2}{dx^2}$ defined on $D(A) = C_0^2(0,1)$, i.e., the $C^2$-functions with compact support inside the open interval $(0,1)$. Both $A_1$ and $A_0$ are bounded below and thus have Friedrichs' extensions. We shall see below that these Friedrichs' extensions are not the same. We will also see that the Friedrichs' extension of $A$ is the same as the Friedrichs' extension of $A_0$.

**PROBLEM 5.18.** *Show that the eigenvalues of the Dirichlet operator $A_0$ in Example 5.17 are $n^2\pi^2$, $n = 1, 2, \ldots$. Show that the eigenvalues of the Neumann operator $A_1$ in Example 5.17 are $n^2\pi^2$, $n = 0, 1, 2, \ldots$. Argue that these operators cannot have the same Friedrichs' extension.*

**PROBLEM 5.19.** *Show that if we consider the operator $A = -\frac{d^2}{dx^2}$ defined on $C_0^2(0,1)$ then the min-max values of $A$ are $\mu_n = n^2\pi^2$ $n = 1, 2, \ldots$. Hence these are eigenvalues of the Friedrichs' extension of $A$. Argue that therefore $A_{\mathrm{F}} = A_{0\mathrm{F}}$. Show however that they are not eigenvalues for the closure of the operator $A$. (From the theory of Fourier series it is known that the eigenfunctions corresponding to the eigenvalues $n^2\pi^2$ $n = 1, 2, \ldots$ form an orthonormal basis for $L^2(0,1)$. You may assume this fact.)*

# 6 The canonical and grand canonical picture and the Fock spaces

We return to the study of the $N$-body operator

$$H_N = H_N^{\rm in} + \sum_{1\leq i<j\leq N} W_{ij} = \sum_{j=1}^N h_j + \sum_{1\leq i<j\leq N} W_{ij} \tag{16}$$

defined on the Hilbert space $\mathcal{H}_N = \mathfrak{h}_1 \otimes \cdots \otimes \mathfrak{h}_N$. This situation where we study a fixed number of particles $N$ is referred to as the *canonical picture*. If we have an infinite sequence of particles (and hence also an infinite sequence of spaces $\mathfrak{h}_1, \mathfrak{h}_2, \ldots$) we may however consider all particle numbers at the same time. To do this we introduce the *Fock* Hilbert space

$$\mathcal{F} = \bigoplus_{N=0}^\infty \mathfrak{h}_1 \otimes \cdots \otimes \mathfrak{h}_N \tag{17}$$

(when $N=0$ we interpret $\mathfrak{h}_1 \otimes \cdots \otimes \mathfrak{h}_N$ as simply $\mathbb{C}$ and refer to it as the 0-particle space, the vector $1 \in \mathbb{C}$ is often called the vacuum vector and is denoted $\Omega$ or $|\Omega\rangle$) and the operator

Correction since May 3: = removed

$$H = \bigoplus_{N=0}^\infty H_N, \quad H \bigoplus_{N=0}^\infty \Psi_N = \bigoplus_{N=0}^\infty H_N \Psi_N \tag{18}$$

(here $H_0 = 0$) with domain

$$D\left(\bigoplus_{N=0}^\infty H_N\right) = \left\{ \Psi = \bigoplus_{N=0}^\infty \Psi_N \mid \Psi_N \in D(H_N),\ \sum_{N=0}^\infty \|H_N\Psi_N\|^2 < \infty \right\}.$$

This situation when all particle numbers are considered at the same time is called the *grand canonical picture*.

**PROBLEM 6.1.** *What is the natural quadratic form domain for $\bigoplus_{N=0}^\infty H_N$?*

**DEFINITION 6.2** (Stability of first and second kind)**.** A many-body system is said to be *stable of the first kind* or *canonically stable* if the operators $H_N$ are stable for all $N$, i.e., if they are bounded below. A many-body system is said to be *stable of the second kind* or *grand canonically stable* if there exists a constant $\mu$ such that the operator

$$\bigoplus_{N=0}^\infty H_N + \mu N$$

(with the same domain as $\bigoplus_{N=0}^\infty H_N$) is stable, i.e., bounded below.

Of special interest is the situation when we have identical particles. In this case we may introduce the bosonic Fock space

$$\mathcal{F}^{\mathrm{B}}(\mathfrak{h}) = \bigoplus_{N=0}^{\infty} \bigotimes_{\mathrm{sym}}^{N} \mathfrak{h} \tag{19}$$

and the fermionic Fock space

$$\mathcal{F}^{\mathrm{F}}(\mathfrak{h}) = \bigoplus_{N=0}^{\infty} \bigwedge^{N} \mathfrak{h}. \tag{20}$$

The projections $P_{\pm}$ defined in (5) may be identified with projections on $\mathcal{F}$ with

$$P_{+}(\mathcal{F}) = \mathcal{F}^{\mathrm{B}}(\mathfrak{h}), \quad P_{-}(\mathcal{F}) = \mathcal{F}^{\mathrm{F}}(\mathfrak{h}).$$

In this case we refer to $\mathfrak{h}$ as the *one-particle space.*

**PROBLEM 6.3.** *Assume we have two one-paticle spaces $\mathfrak{h}_1$ and $\mathfrak{h}_2$. In this problem we shall see that the spaces $\mathcal{F}^{\mathrm{B,F}}(\mathfrak{h}_1 \oplus \mathfrak{h}_2)$ may in a natural way be identified with $\mathcal{F}^{\mathrm{B,F}}(\mathfrak{h}_1) \otimes \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h}_2)$. More precisely, show that there is a unique unitary map*

$$U : \mathcal{F}^{\mathrm{B}}(\mathfrak{h}_1) \otimes \mathcal{F}^{\mathrm{B}}(\mathfrak{h}_2) \to \mathcal{F}^{\mathrm{B}}(\mathfrak{h}_1 \oplus \mathfrak{h}_2)$$

*such that*

$$U(\Phi_1 \otimes \Phi_2) = \sqrt{\frac{(N_1 + N_2)!}{N_1! N_2!}} P_{+}(\Phi_1 \otimes \Phi_2)$$

*for $\Phi_1$ belonging to the $N_1$-particle sector of $\mathcal{F}^{\mathrm{B}}(\mathfrak{h}_1)$ and $\Phi_2$ belonging to the $N_2$-particle sector of $\mathcal{F}^{\mathrm{B}}(\mathfrak{h}_2)$. The corresponding result holds for the fermionic Fock spaces.*

**PROBLEM 6.4.** *Consider an operator of the form $H = \bigoplus_{N=0}^{\infty} H_N$ on $\mathcal{F}$, $\mathcal{F}^{\mathrm{B}}$ or $\mathcal{F}^{\mathrm{F}}$. If $\Psi$ is a normalized vector in the domain $D\left(\bigoplus_{N=0}^{\infty} H_N\right)$ show that there exist $N$ and a normalized vector $\Psi_N \in D(H_N)$ such that $(\Psi, H\Psi) \geq (\Psi_N, H_N \Psi_N)$.*

If we have a system that is stable of the second kind, such that $\bigoplus_{N=0}^{\infty} H_N + \mu N$ is stable, it follows from the above problem that the corresponding ground state energy is always attained at a fixed particle number. The grand canonical picture is useful in situations where we look for the particle number which gives the smallest possible energy.

*EXAMPLE* 6.5 (Molecules). We will here give the quantum mechanical description of a molecule. We first consider the canonical picture where the molecule has $N$ electrons (mass= 1, charge= $-1$, and spin= 1/2) and $K$ nuclei with charges $Z_1, \ldots, Z_K > 0$, masses $M_1, \ldots, M_K$, and spins $j_1, \ldots, j_K$ (satisfying $2j_k + 1 \in \mathbb{N}$ for $k = 1, \ldots, K$). Some nuclei may be identical, but let us for simplicity not treat them as bosons or fermions. The Hilbert space describing the molecule is

$$\mathcal{H}_N = \bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^2) \otimes \bigotimes_{k=1}^K L^2(\mathbb{R}^3; \mathbb{C}^{2j_k+1}).$$

The Hamiltonian is

$$\begin{aligned} H_N \;&=\; \sum_{i=1}^N -\frac{1}{2}\Delta_{x_i} + \sum_{k=1}^K -\frac{1}{2M_k}\Delta_{r_k} + \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|} \\ &\quad - \sum_{i=1}^N \sum_{k=1}^K \frac{Z_k}{|x_i - r_k|} + \sum_{1\le k<\ell\le K} \frac{Z_k Z_\ell}{|r_k - r_\ell|}. \end{aligned}$$

Here we have written the nuclei coordinates as $r_k \in \mathbb{R}^3$, $k = 1, \ldots, K$ and the electron coordinates as $x_i \in \mathbb{R}^3$, $i = 1, \ldots, N$.

We may choose the domain for $H_N$ to be functions in $C_0^2$, i.e., smooth functions with compact support. It can be proved that the molecule is stable in the sense that there is a ground state energy $E_N > -\infty$ (See Problem A.6.1) Correction since May 3: $\infty \to 3$ and problem added

We may now consider the grand canonical picture for the electrons, i.e., we vary the number $N$ of electrons but leave the number $K$ of nuclei fixed. Thus we consider the operator $\bigoplus_{N=0}^\infty H_N$ on the Fock space $\bigoplus_{N=0}^\infty \mathcal{H}_N$. It can be proved that this system is stable of the second kind (even with $\mu = 0$), i.e., that $\inf_N E_N > -\infty$. In fact, there is an $N_c$ such that $E_N = E_{N_c}$ for all $N \ge N_c$. It is known that

$$Z_1 + \ldots + Z_K \le N_c \le 2(Z_1 + \ldots + Z_K) + 1.$$

**PROBLEM 6.6.** *What would the Hilbert space be in the previous example if the nuclei were all identical bosons?*

**PROBLEM 6.7** (Very difficult)**.** *Show that the map $N \mapsto E_N$ defined in the previous example is a non-increasing map.*

*(Hint: Physically adding an electron does not make the ground state energy increasing because we can move this electron to infinity.)* Correction since August 30, 09: Hint added

*EXAMPLE* 6.8 (Matter). In the previous example we considered the number of nuclei fixed, but both the canonical and the grand canonical picture for the electrons. We may also consider the grand canonical situation for the nuclei. Let us assume that we have only a finite number $L$ of different kinds of nuclei and let us still treat them neither as bosons nor fermions. Thus we want to consider an arbitrary number $K$ of nuclei with charges, masses and spins belonging to the set

$$\{(Z_1, M_1, j_1), \ldots, (Z_L, M_L, j_L)\}$$

We have to specify how many of each kind of nuclei we have. Let us not do this explicitly, but only say that as the number of nuclei $K$ tends to infinity we want to have that the fractions of each kind converge to some values $\nu_1, \ldots, \nu_L > 0$ where of course $\nu_1 + \ldots + \nu_L = 1$. Let $E_{N,K}$ be the canonical ground state energy for $N$ electrons and $K$ nuclei. Stability of the second kind for this system states that there is a constant $\mu$ such that

$$E_{N,K} \geq \mu(N + K). \tag{21}$$

This inequality is true. It is called *Stability of Matter*. It was first proved by Dyson and Lenard in 1967–68[10,11] but has a long history in mathematical physics. Moreover, it is true that the limit

$$\lim_{K\to\infty} \frac{\inf_N E_{N,K}}{K}$$

exists. This is a version of what is called *the existence of the thermodynamic limit*. It was proved in a somewhat different form by Lieb and Lebowitz[12].

# 7 Second quantization

We now introduce operators on the bosonic and fermionic Fock spaces that are an important tool in studying many body problems.

[10] Dyson, Freeman J. and Lenard, Andrew, Stability of matter. I, *Jour. Math. Phys.* **8**, 423–434, (1967).

[11] Dyson, Freeman J. and Lenard, Andrew, Stability of matter. II, *Jour. Math. Phys.* **9**, 698–711 (1968).

[12] Lieb, Elliott H. and Lebowitz, Joel L. , The constitution of matter: Existence of thermodynamics for systems composed of electrons and nuclei. Advances in Math. **9**, 316–398 (1972).

For any vector in the one-particle Hilbert space $f \in \mathfrak{h}$. We first introduce two operators $a(f)$ and $a^*(f)$ on the Fock Hilbert space

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N, \quad \mathcal{H}_N = \bigotimes^{N} \mathfrak{h}.$$

These operators are defined by the following actions on the pure tensor products

$$\begin{aligned} a(f)(f_1 \otimes \cdots \otimes f_N) &= N^{1/2}(f, f_1)_{\mathfrak{h}} f_2 \otimes \cdots \otimes f_N \\ a^*(f)(f_1 \otimes \cdots \otimes f_N) &= (N+1)^{1/2} f \otimes f_1 \otimes \cdots \otimes f_N. \end{aligned}$$

On the 0-particle space $\mathbb{C}$ they act as $a(f)\Omega = 0$ and $a^*(f)\Omega = f$. We extend the action of $a(f)$ and $a^*(f)$ by linearity to the domain $\cup_{M=0}^{\infty} \bigoplus_{N=0}^{M} \mathcal{H}_N$. Then $a(f)$ and $a^*(f)$ are densely defined operators in $\mathcal{F}$ with the property that they map

$$a(f) : \mathcal{H}_N \to \mathcal{H}_{N-1}, \quad a^*(f) : \mathcal{H}_N \to \mathcal{H}_{N+1}.$$

We call $a(f)$ an *annihilation* operator and $a^*(f)$ a *creation* operator. We think of $a(f)$ as annihilating a particle in the one-particle state $f$ and of $a^*(f)$ as creating a particle in this state.

**PROBLEM 7.1.** *Show that the operators $a(f)$ and $a^*(f)$ may be extended to the domain*

$$\{\Psi = \bigoplus_{N=0}^{\infty} \Psi_N \mid \sum_{N=0}^{\infty} N\|\Psi_N\|^2 < \infty\}.$$

**PROBLEM 7.2.** *Show that for all vectors $\Psi, \Phi \in \cup_{M=0}^{\infty} \bigoplus_{N=0}^{M} \mathcal{H}_N$ we have*

$$(a(f)\Psi, \Phi)_{\mathcal{F}} = (\Psi, a^*(f)\Phi)_{\mathcal{F}},$$

*when $f \in \mathfrak{h}$. For this reason we say that $a(f)$ and $a^*(f)$ are formal adjoints.*

It is more important to define creation and annihilation operators on the bosonic and fermionic Fock spaces. The annihilation operators may simply be restricted to the bosonic and fermionic subspaces . The creation operators however require that we project back onto the appropriate subspaces using the projections $P_{\pm}$ defined in (5) now considered on the Fock space. Thus we define

$$a_{\pm}(f) = a(f), \quad a_{\pm}^*(f) = P_{\pm} a^*(f) \tag{22}$$

**PROBLEM 7.3.** *Show that $a_\pm(f)$ and $a^*_\pm(f)$ for all vectors $f \in \mathfrak{h}$ define densely defined operators on the spaces $\mathcal{F}^{\mathrm{B}}(\mathfrak{h})$ (in the $+$ case) and $\mathcal{F}^{\mathrm{F}}(\mathfrak{h})$ (in the $-$ case). Show moreover that on their domains these operators satisfy*

$$(a_+(f)\Psi, \Phi)_{\mathcal{F}^{\mathrm{B}}} = (\Psi, a^*_+(f)\Phi)_{\mathcal{F}^{\mathrm{B}}}, \quad (a_-(f)\Psi, \Phi)_{\mathcal{F}^{\mathrm{F}}} = (\Psi, a^*_-(f)\Phi)_{\mathcal{F}^{\mathrm{F}}}.$$

The maps $\mathfrak{h} \ni f \to a^*_\pm(f)$ are linear whereas the maps $\mathfrak{h} \ni f \to a_\pm(f)$ are anti-linear (i.e. conjudate linear).

Correction since August 30, 09: anti-linear=conjugate linear.

**PROBLEM 7.4.** *We introduce the commutator $[A, B] = AB - BA$ and the anti-commutator $\{A, B\} = AB + BA$ of two operators. Show that on their domain of definition the operators $a_+$ and $a^*_+$ satisfy the Canonical Commutation Relations (CCR)*

$$[a_+(f), a_+(g)] = [a^*_+(f), a^*_+(g)] = 0, \quad [a_+(f), a^*_+(g)] = (f, g)_{\mathfrak{h}} I \tag{23}$$

*Show that on their domain of definition the operators $a_-$ and $a^*_-$ satisfy the Canonical Anti-Commutation Relations (CAR)*

$$\{a_-(f), a_-(g)\} = \{a^*_-(f), a^*_-(g)\} = 0, \quad \{a_-(f), a^*_-(g)\} = (f, g)_{\mathfrak{h}} I. \tag{24}$$

**PROBLEM 7.5.** *Show that if $\dim \mathfrak{h} = n$ then $\dim(\mathcal{F}^{\mathrm{F}}(\mathfrak{h})) = 2^n$. If $e_1, \ldots, e_n$ are orthonormal basis vectors in $\mathfrak{h}$ describe the action of the operators $a_-(e_i), a^*_-(e_i)$ on an appropriate basis in $\mathcal{F}^{\mathrm{F}}(\mathfrak{h})$.*

**PROBLEM 7.6.** *In this exercise we will give two descriptions of the Fock space $\mathcal{F}^{\mathrm{B}}(\mathbb{C})$.*

*Show that $\mathcal{F}^{\mathrm{B}}(\mathbb{C})$ in a natural way may be identified with the space $\ell^2(\mathbb{N})$ such that the vacuum vector $\Omega$ is the sequence $(1, 0, 0, 0 \ldots)$. Let $|n\rangle$ denote the sequence with 1 in the n-th position and 0 elsewhere. Write the actions of the operators $a_+(1), a^*_+(1)$ on the basis vector $|n\rangle$.*

Correction since May 3 vacuum vector normalization corrected

*Show that we may also identify $\mathcal{F}^{\mathrm{B}}(\mathbb{C})$ with the space $L^2(\mathbb{R})$ such that the vacuum vector $\Omega$ is the function $(\pi)^{-1/4}e^{-x^2/2}$ and $a_+(1) = \frac{1}{\sqrt{2}}(x + \frac{d}{dx})$, $a^*_+(1) = \frac{1}{\sqrt{2}}(x - \frac{d}{dx})$. For this last question it is useful to know that the space of functions of the form $p(x)e^{-x^2/2}$, where $p(x)$ is a polynomial, is a dense subspace in $L^2(\mathbb{R})$.*

**PROBLEM 7.7.** 1. *Show that if $u \in \mathfrak{h}$ is a unit vector then we have a direct sum decomposition $\mathcal{F}^{\mathrm{B}}(\mathfrak{h}) = \bigoplus_{n=0}^\infty \mathcal{H}_n$ such that $\mathcal{H}_n$ is an eigenspace of eigenvalue $n$ for the operator $a^*_+(u)a_+(u)$.*

2. *If $u_1,\ldots,u_r\in\mathfrak{h}$ are orthonormal vectors then we have a direct sum decomposition $\mathcal{F}^{\rm B}(\mathfrak{h})=\bigoplus_{n_1=0}^{\infty}\cdots\bigoplus_{n_r=0}^{\infty}\mathcal{H}_{n_1,\ldots,n_r}$ such that $\mathcal{H}_{n_1,\ldots,n_r}$ is a joint eigenspace for the operators $a_+^*(u_1)a_+(u_1),\ldots,\ a_+^*(u_r)a_+(u_r)$ of eigenvalues $n_1,\ldots,n_r$ respectively.*

3. *Likewise for fermions show that if $u_1,\ldots,u_r\in\mathfrak{h}$ are orthonormal vectors then we have a direct sum decomposition $\mathcal{F}^{\rm F}(\mathfrak{h})=\bigoplus_{n_1=0}^{1}\cdots\bigoplus_{n_r=0}^{1}\mathcal{H}_{n_1,\ldots,n_r}$ such that $\mathcal{H}_{n_1,\ldots,n_r}$ is a joint eigenspace (i.e. the intersections of eigenspaces) for the operators $a_-^*(u_1)a_-(u_1),\ldots,\ a_-^*(u_r)a_-(u_r)$ with eigenvalues $n_1,\ldots,n_r$ respectively.*

Correction since August 30, 09: Definition of joint spaces is added.

**LEMMA 7.8** (2nd quantization of 1-body operator)**.** *Let $h$ be a symmetric operator on $\mathfrak{h}$ and let $\{u_\alpha\}_{\alpha=1}^{\infty}$ be an orthonormal basis for $\mathfrak{h}$ with elements from the domain $D(h)$. We may then write*

$$\bigoplus_{N=1}^{\infty}\sum_{j=1}^{N}h_j=\sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty}(u_\alpha,hu_\beta)a_\pm^*(u_\alpha)a_\pm(u_\beta) \qquad (25)$$

*as quadratic forms on the domain $\cup_{M=0}^{\infty}\bigoplus_{N=1}^{M}P_\pm D(\sum_{j=1}^{N}h_j)$ (for $M=0$ the domain is $\mathbb{C}$).*

*Proof.* We first observe that if $f,g\in D(h)$ then

$$\begin{aligned}\sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty}(g,u_\alpha)_{\mathfrak{h}}(u_\alpha,hu_\beta)_{\mathfrak{h}}(u_\beta,f)_{\mathfrak{h}} &= \sum_{\beta=1}^{\infty}(g,hu_\beta)_{\mathfrak{h}}(u_\beta,f)_{\mathfrak{h}}=\sum_{\beta=1}^{\infty}(hg,u_\beta)_{\mathfrak{h}}(u_\beta,f)_{\mathfrak{h}}\\ &= (hg,f)_{\mathfrak{h}}=(g,hf)_{\mathfrak{h}}.\end{aligned}$$

This in fact shows that the identity (25) holds in the sense of quadratic forms on $D(h)$.

Let us consider the action of $a^*(u_\alpha)a(u_\beta)$ on a pure tensor product

$$a^*(u_\alpha)a(u_\beta)f_1\otimes\cdots\otimes f_N=N(u_\beta,f_1)_{\mathfrak{h}}u_\alpha\otimes f_2\otimes\cdots\otimes f_N$$

where $f_1,\ldots,f_N\in D(h)$. Thus we have

$$\sum_{\beta=1}^{\infty}\sum_{\alpha=1}^{\infty}(u_\alpha,hu_\beta)_{\mathfrak{h}}a^*(u_\alpha)a(u_\beta)=Nh_1$$

as quadratic forms on finite linear combinations of $N$-fold pure tensor products of vectors from $D(h)$.

Correction since August 30, 09: functions → vectors.

Since $P_\pm$ projects onto symmetrized or anti-symmetrized vectors we have $P_\pm N h_1 P_\pm = P_\pm \sum_{j=1}^N h_j P_\pm = \sum_{j=1}^N h_j P_\pm$ on $\bigotimes^N \mathfrak{h}$. Hence

$$\begin{aligned}\sum_{\beta=1}^\infty\sum_{\alpha=1}^\infty (u_\alpha, h u_\beta)_{\mathfrak{h}} a_\pm^*(u_\alpha) a_\pm(u_\beta) P_\pm &= \sum_{\beta=1}^\infty\sum_{\alpha=1}^\infty (u_\alpha, h u_\beta)_{\mathfrak{h}} P_\pm a^*(u_\alpha) a(u_\beta) P_\pm \\ &= \bigoplus_{N=1}^\infty \sum_{j=1}^N h_j P_\pm .\end{aligned}$$

□

**DEFINITION 7.9** (2nd quantization of 1-body operator)**.** The operator

$$\bigoplus_{N=1}^\infty \sum_{j=1}^N h_j$$

is called the second quantization of the operator $h$. It is sometimes denoted $d\Gamma(h)$, but we will not use this notation here.

*REMARK* 7.10. If $U$ is an operator on $\mathfrak{h}$ another way to lift $U$ to the Fock space $\mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$ is muliplicatively

$$\Gamma(U) = \bigoplus_{N=0}^\infty \bigotimes^N U$$

($\bigotimes^N U = I$ when $N = 0$.) This is also denoted the second quantization of $U$. It is the relevant operation for transformation operators, e.g., unitary maps.

Correction since May 3: Case $N = 0$ added

**PROBLEM 7.11.** *Show that one can always find an orthonormal basis for $\mathfrak{h}$ consisting of vectors from a given dense subspace.*

Note that the second quantization of the identity operator $I$ on $\mathfrak{h}$ is the number operator $\mathcal{N} = \bigoplus_{N=0}^\infty N$ on $\mathcal{F}^{\mathrm{B}}(\mathfrak{h})$ or $\mathcal{F}^{\mathrm{F}}(\mathfrak{h})$. The number operator may be written as

$$\mathcal{N} = \sum_{\alpha=1}^\infty a_\pm^*(u_\alpha) a_\pm(u_\alpha), \tag{26}$$

for any orthonormal basis $\{u_\alpha\}_{\alpha=1}^\infty$ on $\mathfrak{h}$.

We have a similar result for 2-body potentials.

**LEMMA 7.12** (2nd quantization of 2-body operator)**.** *Let $\{u_\alpha\}_{\alpha=1}^\infty$ be an orthonormal basis for $\mathfrak{h}$. Let $W$ be a 2-body potential for identical particles, i.e., a symmetric operator on $\mathfrak{h}\otimes\mathfrak{h}$ such that $\mathrm{Ex}W\mathrm{Ex} = W$. Assume that $u_\alpha\otimes u_\beta \in D(W)$ for all $\alpha,\beta = 1,2,\ldots$. Then as quadratic forms on finite linear combinations of pure symmetric (+) or antisymmetric (-) tensor products of basis vectors from $\{u_\alpha\}_{\alpha=1}^\infty$ we have*

$$\bigoplus_{N=2}^\infty \sum_{1\leq i<j\leq N} W_{ij} = \tfrac{1}{2}\sum_{\alpha,\beta,\mu,\nu=1}^\infty (u_\alpha\otimes u_\beta, Wu_\mu\otimes u_\nu)a_\pm^*(u_\alpha)a_\pm^*(u_\beta)a_\pm(u_\nu)a_\pm(u_\mu). \tag{27}$$

*Proof.* We have

$$Wu_1\otimes u_2 = \sum_{\alpha,\beta,\mu,\nu=1}^\infty (u_\alpha\otimes u_\beta, Wu_\mu\otimes u_\nu)_{\mathfrak{h}\otimes\mathfrak{h}}(u_\mu,u_1)_{\mathfrak{h}}(u_\nu,u_2)_{\mathfrak{h}}u_\alpha\otimes u_\beta$$

and

$$\begin{aligned}&a^*(u_\alpha)a^*(u_\beta)a(u_\nu)a(u_\mu)u_1\otimes u_2\otimes\cdots\otimes u_N = \\ &\quad N(N-1)(u_\mu,u_1)(u_\nu,u_2)u_\alpha\otimes u_\beta\otimes u_3\otimes\cdots\otimes u_N.\end{aligned}$$

Since this is true for any $N$-fold pure tensor product of basis vectors we conclude that on such tensor products

$$\tfrac{1}{2}\sum_{\alpha,\beta,\mu,\nu=1}^\infty (u_\alpha\otimes u_\beta, Wu_\mu\otimes u_\nu)a^*(u_\alpha)a^*(u_\beta)a(u_\nu)a(u_\mu) = \frac{N(N-1)}{2}W_{12}.$$

As in the previous proof we have that on $N$-fold tensor products

$$\frac{N(N-1)}{2}P_\pm W_{12}P_\pm = \sum_{1\leq i<j\leq N} W_{ij}P_\pm$$

(we are here using that $\mathrm{Ex}W\mathrm{Ex} = W$). Note that $P_\pm a^*(f)P_\pm = P_\pm a^*(f)$ (if we symmetrize or anti-symmetrize after creating an extra particle it plays no role whether we had symmetrized or anti-symmetrized before). Thus

$$\begin{aligned}\bigoplus_{N=2}^\infty \sum_{1\leq i<j\leq N} W_{ij}P_\pm &= \bigoplus_{N=2}^\infty \frac{N(N-1)}{2}P_\pm W_{12}P_\pm \\ &= P_\pm\tfrac{1}{2}\sum_{\alpha,\beta,\mu,\nu=1}^\infty (u_\alpha\otimes u_\beta, Wu_\mu\otimes u_\nu)a^*(u_\alpha)a^*(u_\beta)a(u_\nu)a(u_\mu)P_\pm\end{aligned}$$

$$= \tfrac{1}{2} \sum_{\alpha,\beta,\mu,\nu=1}^{\infty} (u_\alpha \otimes u_\beta, W u_\mu \otimes u_\nu) P_\pm a^*(u_\alpha) P_\pm a^*(u_\beta) a(u_\nu) a(u_\mu) P_\pm$$
$$= \tfrac{1}{2} \sum_{\alpha,\beta,\mu,\nu=1}^{\infty} (u_\alpha \otimes u_\beta, W u_\mu \otimes u_\nu) a_\pm^*(u_\alpha) a_\pm^*(u_\beta) a_\pm(u_\nu) a_\pm(u_\mu) P_\pm.$$

□

**DEFINITION 7.13** (2nd quantization of 2-body operator)**.** The operator

$$\bigoplus_{N=2}^{\infty} \sum_{1\le i<j\le N} W_{ij}$$

is called the second quantization of the two-body operator $W$.

# 8 One- and two-particle density matrices for bosonic or fermionic states

**DEFINITION 8.1** (One-particle density matrix)**.** Let $\Psi = \bigoplus_{N=0}^{\infty} \Psi_N$ be a normalized vector on the bosonic Fock space $\mathcal{F}^{\mathrm{B}}(\mathfrak{h})$ or the fermionic Fock space $\mathcal{F}^{\mathrm{F}}(\mathfrak{h})$ with finite particle expectation

Correction since May 3: Formula for $\Psi$ corrected

$$(\Psi, \mathcal{N}\Psi) = \sum_{N=0}^{\infty} N \|\Psi_N\|^2 < \infty.$$

We define the 1-particle density matrix (or 2-point function) of $\Psi$ as the operator $\gamma_\Psi$ on the one-body space $\mathfrak{h}$ given by

$$(f, \gamma_\Psi g)_{\mathfrak{h}} = (\Psi, a_\pm^*(g) a_\pm(f) \Psi).$$

**PROBLEM 8.2.** *Show that $\gamma_\Psi$ is a positive semi-definite trace class operator with*

$$\mathrm{Tr}\gamma_\Psi = (\Psi, \mathcal{N}\Psi).$$

**PROBLEM 8.3.** *Show that if $\Psi$ is a finite linear combination of pure tensor products of elements from a subspace $X \subseteq \mathfrak{h}$ then $\gamma_\Psi$ is a finite rank operator whose range is a subspace of $X$.*

**THEOREM 8.4** (Fermionic 1-particle density matrix)**.** *If $\Psi$ is a normalized vector on the fermionic Fock space $\mathcal{F}^{\mathrm{F}}(\mathfrak{h})$ then $\gamma_\Psi$ satisfies the operator inequality*

$$0 \leq \gamma_\Psi \leq I. \tag{28}$$

*In particular, the eigenvalues of $\gamma_\Psi$ are in the interval $[0,1]$.*

*Proof.* We simply have to prove that for all $f \in \mathfrak{h}$ we have

$$0 \leq (f, \gamma_\Psi f)_{\mathfrak{h}} \leq \|f\|^2.$$

The first inequality follows from Problem 7.3 since

$$(f, \gamma_\Psi f)_{\mathfrak{h}} = (\Psi, a_-^*(f) a_-(f)\Psi) = (a_-(f)\Psi, a_-(f)\Psi) = \|a_-(f)\Psi\|^2 \geq 0.$$

The second inequality above follows from Problem 7.3 and the CAR relations (24) since

$$\begin{aligned}(f, \gamma_\Psi f)_{\mathfrak{h}} &= (\Psi, a_-^*(f) a_-(f)\Psi) \leq (\Psi, a_-^*(f) a_-(f)\Psi) + (a_-^*(f)\Psi, a_-^*(f)\Psi) \\ &= (\Psi, a_-^*(f) a_-(f) + a_-(f) a_-^*(f)\Psi) = (\Psi, \{a_-(f), a_-^*(f)\}\Psi) = \|f\|^2.\end{aligned}$$

□

**PROBLEM 8.5.** *If $u_1, \ldots, u_N$ are orthonormal vectors in $\mathfrak{h}$ we consider the normalized (see Problem 1.24) vector $\Psi = u_1 \wedge \cdots \wedge u_N$. Show that the corresponding 1-particle density matrix $\gamma_\Psi$ is the projection in $\mathfrak{h}$ onto the $N$-dimensional space spanned by $u_1, \ldots, u_N$.*

We are now ready to prove the result corresponding to Corollary 2.10 for fermions.

**THEOREM 8.6** (Ground state of non-interacting Fermi system)**.** *We consider the Hamiltonian $H_N^{\mathrm{in}} = \sum_{j=1}^N h_j$ for $N$ identical particles restricted to the anti-symmetric subspace $\bigwedge^N \mathfrak{h}$, i.e., with domain*

$$D_-(H_N^{\mathrm{in}}) = P_- D(H_N^{\mathrm{in}}).$$

*We assume that the one-body operator $h$ is bounded from below. The ground state energy of this fermionic system is*

$$\inf\{\mathrm{Tr}(Ph) \mid P \text{ an orth. projection onto an } N\text{-dimensional subspace of } D(h)\}. \tag{29}$$

*If the infimum is attained for an $N$-dimensional projection $P$ then $H_N^{\rm in}$ has a ground state eigenvector $f_1 \wedge \cdots \wedge f_N$, where $f_1, \ldots, f_N$ is an orthonormal basis for the space $P(\mathfrak{h})$. This basis may be chosen to consist of eigenvectors of $h$. All expectations of $h$ restricted to the orthogonal complement $P(\mathfrak{h})^\perp \cap D(h)$ will be greater than all expectations of $h$ restricted to $P(\mathfrak{h})$.*

Notice that according to Problem 4.13 the ground state energy of the $N$-particle fermionic system may be described as $\sum_{n=1}^N \mu_n(h)$, where $\mu_n(h)$ are the min-max values of $h$.

*Proof.* Choose an orthonormal basis $\{u_\alpha\}_{\alpha=1}^\infty$ for $\mathfrak{h}$ with vectors from $D(h)$ (see Problem 7.11) Let $\Psi \in D_-(H_N^{\rm in})$ be normalized. It follows from Lemma 7.8 that

$$(\Psi, H_N^{\rm in}\Psi) = \sum_{\beta=1}^\infty \sum_{\alpha=1}^\infty (u_\alpha, hu_\beta)(\Psi, a_-^*(u_\alpha)a_-(u_\beta)\Psi) = \sum_{\beta=1}^\infty \sum_{\alpha=1}^\infty (u_\alpha, hu_\beta)(u_\beta, \gamma_\Psi u_\alpha).$$

Recall that $\Psi$ is assumed to be a finite linear combination of pure tensor products of elements from $D(h)$. Thus from Problem 8.3 we know that $\gamma_\Psi$ has finite rank. Let $\gamma_\Psi$ have eigenvectors $v_1, \ldots, v_n$ and corresponding eigenvalues $\lambda_1, \ldots, \lambda_n$. It follows again from Problem 8.3 that $v_1, \ldots, v_n \in D(h)$. Then

$$(\Psi, H_N^{\rm in}\Psi) = \sum_{j=1}^n \sum_{\beta=1}^\infty \sum_{\alpha=1}^\infty \lambda_j (u_\alpha, hu_\beta)(u_\beta, v_j)(v_j, u_\alpha) = \sum_{j=1}^n \lambda_j (v_j, hv_j)$$

The state $\Psi$ has fixed particle number $N$ therefore we have that

$$\sum_{j=1}^n \lambda_j = {\rm Tr}\gamma_\Psi = (\Psi, \mathcal{N}\Psi) = N.$$

Since $0 \leq \lambda_j \leq 1$ we must have $n \geq N$.

We may assume that we had chosen the eigenvectors ordered such that

$$(v_1, hv_1) \leq (v_2, hv_2) \leq \ldots \leq (v_n, hv_n).$$

If we define the $N$-dimensional projection $P$ that projects onto the space spanned by $v_1, \ldots, v_N$ we find that

$${\rm Tr}[Ph] = \sum_{j=1}^N (v_j, hv_j) \leq \sum_{j=1}^n \lambda_j (v_j, hv_j) \leq (\Psi, H_N^{\rm in}\Psi).$$

Thus

$$\inf\{\mathrm{Tr}(Ph) \mid P \text{ an orth. projection onto an N-dimensional subspace of } D(h)\}$$
$$\leq \inf\{(\Psi, H_N^{\mathrm{in}}\Psi) \mid \Psi \in D(H_N^{\mathrm{in}}), \|\Psi\| = 1\}$$

The opposite inequality is also true. In fact, given $N$ orthonormal vectors $f_1, \ldots, f_N \in D(h)$. Let $\Psi = f_1 \wedge \cdots \wedge f_N$. Then according to Problem 8.5 $\gamma_\Psi = P$ is the projection onto the space spanned by $f_1, \ldots, f_N$. As above we find that $(\Psi, H_N^{\mathrm{in}}\Psi) = \mathrm{Tr}[Ph]$.

Assume now that $P$ minimizes the variational problem in (29). It is clear from the above proof that the vector $\Psi = f_1 \wedge \cdots \wedge f_N$ is a ground state for $H_N^{\mathrm{in}}$ if $f_1, \ldots, f_N$ is an orthonormal basis for $P(\mathfrak{h})$.

We now show the stated properties of the space $P(\mathfrak{h})$ corresponding to a minimizing projection.

It is first of all clear that if $\phi \in P(\mathfrak{h})$ and $\psi \in P(\mathfrak{h})^\perp \cap D(h)$ are normalized then

$$(\phi, h\phi) \leq (\psi, h\psi).$$

In fact, consider the projection $Q$ onto the $N$-dimensional space

$$\mathrm{span}(P(\mathfrak{h}) \cap \{\phi\}^\perp) \cup \{\psi\},$$

i.e., the space where we have replaced $\phi$ by $\psi$. We then have since $P$ is minimizing

$$0 \leq \mathrm{Tr}[Qh] - \mathrm{Tr}[Ph] = (\psi, h\psi) - (\phi, h\phi).$$

The same argument actually shows that if $\psi \in D(h) \cap (P(\mathfrak{h}) \cap \{\phi\}^\perp)^\perp$ is normalized then $(\phi, h\phi) \leq (\psi, h\psi)$. We will now use this to show that $h$ maps the space $P(\mathfrak{h})$ into itself. Assume otherwise, that there is a $\phi \in P(\mathfrak{h})$ such that $h\phi \notin P(\mathfrak{h})$. Since $D(h)$ is dense there is a $g \in D(h)$ such that $((I - P)g, h\phi) = (g, (I - P)h\phi) \neq 0$. Assume that $\mathrm{Re}((I - P)g, h\phi) \neq 0$ (otherwise we simply multiply $g$ by $i$). We have $(I - P)g \in D(h)$. Consider for $t \in \mathbb{R}$ (close to 0)

$$\phi_t = \frac{\phi + t(I - P)g}{\|\phi + t(I - P)g\|}.$$

Note that $\phi_t \in D(h) \cap (P(\mathfrak{h}) \cap \{\phi\}^\perp)^\perp$. Hence $(\phi, h\phi) \leq (\phi_t, h\phi_t)$. This is however in contradiction with the fact that

$$\frac{d}{dt}(\phi_t, h\phi_t)_{|t=0} = ((I - P)g, h\phi) + (\phi, h(I - P)g) = 2\mathrm{Re}((I - P)g, h\phi) \neq 0.$$

Thus $h$ maps $P(\mathfrak{h})$ to itself and this space is hence spanned by eigenvectors of $h$. $\square$

**PROBLEM 8.7** (Bosonic 1-particle density matrix). *If $\phi \in \mathfrak{h}$ is normalized we consider the $N$-fold tensor product of $\phi$ with itself $\Psi = \phi \otimes \phi \otimes \cdots \phi$. Note that $\Psi \in \bigotimes_{\mathrm{sym}}^N \mathfrak{h} \subseteq \mathcal{F}^{\mathrm{B}}(\mathfrak{h})$. Determine the 1-particle density matrix $\gamma_\Psi$.*

## 8.1 Two-particle density matrices

**DEFINITION 8.8** (Two-particle density matrix). Let $\Psi = \bigoplus_{N=0}^\infty \Psi_N$ be a normalized vector on the bosonic Fock space $\mathcal{F}^{\mathrm{B}}(\mathfrak{h})$ or the fermionic Fock space $\mathcal{F}^{\mathrm{F}}(\mathfrak{h})$ with

Correction since August 30, 09: $\bigoplus_{N=0}^\infty \to \bigoplus_{N=0}^\infty \Psi_N$.

$$(\Psi, \mathcal{N}^2\Psi) = \sum_{N=0}^\infty N^2 \|\Psi_N\|^2 < \infty.$$

We define the 2-particle density matrix (or 4-point function) of $\Psi$ as the operator $\Gamma_\Psi^{(2)}$ on the two-body space $\mathfrak{h} \otimes \mathfrak{h}$ uniquely given by

$$(f_1 \otimes f_2, \Gamma_\Psi^{(2)} g_1 \otimes g_2)_{\mathfrak{h}\otimes\mathfrak{h}} = (\Psi, a_\pm^*(g_2) a_\pm^*(g_1) a_\pm(f_1) a_\pm(f_2)\Psi). \tag{30}$$

(in the fermionic case the ordering of the creation and annihilation operators is important).

Correction since June 24: equation number added, problem reformulated

**PROBLEM 8.9.** *Show that (30) indeed uniquely defines a positive semi-definite trace class operator $\Gamma_\Psi^{(2)}$ is with*

$$\mathrm{Tr}\Gamma_\Psi^{(2)} = (\Psi, \mathcal{N}(\mathcal{N}-1)\Psi).$$

*Show also that*

$$\mathrm{Ex}\Gamma_\Psi^{(2)} = \pm\Gamma_\Psi^{(2)} \tag{31}$$

*where $(+)$ is for bosons and $(-)$ is for fermions The exchange operator* Ex *was defined on Page 9.*

**PROBLEM 8.10.** *(Compare Problem 8.5) If $u_1, \ldots, u_N$ are orthonormal vectors in $\mathfrak{h}$ we consider the normalized (see Problem 1.24) vector $\Psi = u_1 \wedge \cdots \wedge u_N$. Show that the corresponding 2-particle density matrix $\Gamma_\Psi^{(2)}$ is given by*

$$\Gamma_\Psi^{(2)} = \gamma_\Psi \otimes \gamma_\Psi - \mathrm{Ex}\gamma_\Psi \otimes \gamma_\Psi$$

*(see Page 9 for the definition of the tensor product of operators). Determine the eigenvectors and eigenvalues of* $\Gamma_\Psi^{(2)}$ *and conclude, in particular, that the largest eigenvalue of* $\Gamma_\Psi^{(2)}$ *is at most 2.*

Correction since May 3 $1 \to 2$

**PROBLEM 8.11** (Bosonic 2-particle density matrix)**.** *Determine the 2-particle density matrix for the bosonic state in Problem 8.7.*

**THEOREM 8.12** (Fermionic 2-particle density matrix)**.** *If* $\dim \mathfrak{h} = M$ *and* $\Psi \in \bigwedge^N \mathfrak{h}$ *for some* $N \leq M$ *and* $\Psi$ *is normalized then if* $N$ *and* $M$ *are even*

$$0 \leq \Gamma_\Psi^{(2)} \leq \frac{N(M-N+2)}{M} I. \tag{32}$$

*For all* $M$ *including* $M = \infty$ *we have*

Correction since May 3: Last sentence of lemma improved

$$0 \leq \Gamma_\Psi^{(2)} \leq NI. \tag{33}$$

*REMARK* 8.13.

- For $N = 2$ the upper bound in (32) is equal to the simple bound $\Gamma_\Psi^{(2)} \leq N(N-1)I$, which follows from Problem 8.9. For all $N > 2$ the bound in (32) is strictly smaller than the simple bound. (This is left for the reader to check.)
- If $N = M$ the upper bound in (32) is $\Gamma_\Psi^{(2)} \leq 2I$. Only in this case does the upper bound in (32) agree with the upper bound for Slater determinants (see Problem 8.10).
- We shall see in the proof of Theorem 8.12 that the upper bound in (32) is achieved for special pair states, in which certain pairs of states are either both occupied or both empty. This is an example of what is called *Cooper* pairs and states of this type was very important in the famous Bardeen-Cooper-Schrieffer theory of superconductivity[13]

Correction since May 3: there → their

- A discussion of other results on bounds of 1-,2- and $n$-point functions and their relations to physics may be found in a classical paper of C.N. Yang[14]

In order to prove the above theorem we need a little lemma.

Correction since May 3: Lemma formulation corrected

[13] J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Theory of Superconductivity, *Phys. Rev.*, **108**, 1175–1204 (1957).

[14] C.N. Yang, Concept of Off-Diagonal Long Range Order and the Quantum Phases of Liquid He and of Superconductors, *Rev. of Mod. Phys.*, **34**, 694–704, 1962.

**LEMMA 8.14.** *If* $\dim(\mathfrak{h}) = M$ *and* $f \in \mathfrak{h} \wedge \mathfrak{h}$ *there exist orthonormal vectors* $u_1, \ldots, u_{2r}$*, where* $r$ *is a positive integer less than or equal to* $M/2$ *and* $\lambda_1, \ldots, \lambda_r \geq 0$ *such that*

Correction since August 30, 09: "less than" → "less than or equal to".

$$f = \sum_{i=1}^{r} \lambda_i u_{2i-1} \wedge u_{2i} = \lambda_1 u_1 \wedge u_2 + \lambda_2 u_3 \wedge u_4 + \ldots.$$

This lemma is proved in Appendix E.

*Proof of Theorem 8.12.* (See also Appendix A in the paper by C.N.Yang in footnote 14.) We will write $M = 2m$ and $N = 2n$ where $m, n$ are positive integers. We will proceed by induction on $M$. If $M = 2$ then $N$ must be 2 (the case $N = 0$ is trivial). If $u_1, u_2$ is an orthonormal basis for $M$ then the only possible state with two particles is $\Psi = u_1 \wedge u_2$. This is the case studied in Problem 8.10, where we saw that indeed the largest eigenvalue is $2 = \frac{N(M-N+2)}{M}$. The same argument actually may be used whenever $M = N$.

Assume now that $M > 2$ and $N < M - 2$ and that the theorem has been proved for $M - 2$ and all $N \leq M - 2$.

Let $f \in \mathfrak{h} \otimes \mathfrak{h}$ and $\Psi \in \bigwedge^N \mathfrak{h}$ be normalized vectors such that $(f, \Gamma_\Psi^{(2)} f)_{\mathfrak{h}\otimes\mathfrak{h}}$ is as large as possible. Then similarly to Problem 2.5 we conclude that $f$ is an eigenvector of $\Gamma_\Psi^{(2)}$. As a consequence of (31) $f$ is antisymmetric, i.e., $f \in \mathfrak{h} \wedge \mathfrak{h}$. According to Lemma 8.14 we may write

$$f = \sum_{i=1}^{m} \lambda_i u_{2i-1} \wedge u_{2i}.$$

Let $a_i = a_-(u_i)$ hence $a_i^* = a_-^*(u_i)$. Define

$$F = \sum_{i=1}^{m} \sqrt{2}\lambda_i a_{2i-1} a_{2i}.$$

The definition of $\Gamma_\Psi^{(2)}$ implies that

$$(f, \Gamma_\Psi^{(2)} f)_{\mathfrak{h}\otimes\mathfrak{h}} = (\Psi, F^* F \Psi)_{\mathcal{F}^{\mathrm{F}}(\mathfrak{h})}. \tag{34}$$

Since $f$ is normalized, i.e., $\sum_{i=1}^m \lambda_i^2 = 1$ we may without loss of generality assume that $\lambda_1 > 0$. Let us introduce $F' = \sum_{i=2}^m \sqrt{2}\lambda_i a_{2i-1} a_{2i}$ such that $F = F' + \sqrt{2}\lambda_1 a_1 a_2$. Then

$$F^* F = F'^* F' + \sqrt{2}\lambda_1 F'^* a_1 a_2 + \sqrt{2}\lambda_1 a_2^* a_1^* F' + 2\lambda_1^2 a_2^* a_1^* a_1 a_2 \tag{35}$$

We write

$$\Psi = \Phi_{00} + \Phi_{01} + \Phi_{10} + \Phi_{11},$$

corresponding to the direct sum decomposition described in Problem 7.7(3) for the operators $a_1^* a_1$ and $a_2^* a_2$, i.e., $\Phi_{k\ell}$ for $k, \ell = 0, 1$ is the projection of $\Psi$ onto the subspace where the number of particles in states $u_1$ and $u_2$ are $k$ and $\ell$ or more explicitly

$$a_1^* a_1 \Phi_{k\ell} = k\Phi_{k\ell}, \quad \text{and} \quad a_2^* a_2 \Phi_{k\ell} = \ell\Phi_{k\ell}.$$

From (35) we obtain

$$\begin{aligned}
(\Psi, F^* F \Psi) &= (\Phi_{00}, F'^* F' \Phi_{00}) + (\Phi_{01}, F'^* F' \Phi_{01}) + (\Phi_{10}, F'^* F' \Phi_{10}) \\
&\quad + (\Phi_{11}, (F'^* F' + 2\lambda_1^2 a_2^* a_1^* a_1 a_2)\Phi_{11}) \\
&\quad + (\Phi_{00}, \sqrt{2}\lambda_1 F'^* a_1 a_2 \Phi_{11}) + (\Phi_{11}, \sqrt{2}\lambda_1 a_2^* a_1^* F' \Phi_{00}) \\
&= (\Phi_{00}, F'^* F' \Phi_{00}) + (\Phi_{01}, F'^* F' \Phi_{01}) + (\Phi_{10}, F'^* F' \Phi_{10}) \\
&\quad + (\Phi_{11}, F'^* F' \Phi_{11}) + 2\lambda_1^2 (\Phi_{11}, \Phi_{11}) \\
&\quad + \sqrt{2}\lambda_1 (\Phi_{00}, F'^* a_1 a_2 \Phi_{11}) + (\Phi_{11}, \sqrt{2}\lambda_1 a_2^* a_1^* F' \Phi_{00}).
\end{aligned}$$

We observe that this expression is a sum of two quadratic forms

$$(\Psi, F^* F \Psi) = Q_1(\Phi_{00} + \Phi_{11}) + Q_2(\Phi_{01} + \Phi_{10}).$$

We will now argue that without decreasing the value of $(\Psi, F^* F \Psi)$ we may assume that either $\Phi_{00} = \Phi_{11} = 0$ or $\Phi_{01} = \Phi_{10} = 0$. In fact, if this were not already the case we would have

Correction since August 30, 09: changing $\to$ decreasing.

$$(\Psi, F^* F \Psi) \leq \max\left\{ \frac{Q_1(\Phi_{00} + \Phi_{11})}{\|\Phi_{00}\|^2 + \|\Phi_{11}\|^2}, \frac{Q_2(\Phi_{01} + \Phi_{10})}{\|\Phi_{01}\|^2 + \|\Phi_{10}\|^2} \right\},$$

i.e., we would do just as well by choosing either $\Phi_{00} = \Phi_{11} = 0$ or $\Phi_{01} = \Phi_{10} = 0$.

Correction since May 3: $01 \to 10$

Since $Q_2$ does not depend on $\lambda_1$ we see that the best choice cannot be $\Phi_{00} = \Phi_{11} = 0$ because in this case we could increase the value of $Q_2(\Phi_{01} + \Phi_{10})$ to $(1-\lambda_1^2)^{-1} Q_2(\Phi_{01} + \Phi_{10})$ by replacing $f$ by $f' = (1-\lambda_1^2)^{-1/2} \sum_{i=2}^r \lambda_i u_{2i-1} \wedge u_{2i}$ in contradiction with the fact that the value was already chosen optimal. Therefore we may assume that $\Phi_{01} = \Phi_{10} = 0$.

Correction since May 3: Explanation of $\Phi_{01} = \Phi_{10} = 0$ improved

We therefore have

$$\begin{aligned}
(\Psi, F^* F \Psi) &= (\Phi_{00}, F'^* F' \Phi_{00}) + (\Phi_{11}, F'^* F' \Phi_{11}) + 2\lambda_1^2 (\Phi_{11}, \Phi_{11}) \\
&\quad + \sqrt{2}\lambda_1 (\Phi_{00}, F'^* a_1 a_2 \Phi_{11}) + (\Phi_{11}, \sqrt{2}\lambda_1 a_2^* a_1^* F' \Phi_{00}).
\end{aligned}$$

We will now apply the Cauchy-Schwarz inequality

$$\begin{aligned}
&(\Phi_{00}, F'^* a_1 a_2 \Phi_{11}) + (\Phi_{11}, a_2^* a_1^* F' \Phi_{00}) \\
&\quad = (F'\Phi_{00}, a_1 a_2 \Phi_{11}) + (a_1 a_2 \Phi_{11}, F'\Phi_{00}) \\
&\quad \leq 2(a_1 a_2 \Phi_{11}, a_1 a_2 \Phi_{11})^{1/2} (\Phi_{00}, F'^* F' \Phi_{00})^{1/2} \\
&\quad \leq 2(\Phi_{11}, a_2^* a_1^* a_1 a_2 \Phi_{11})^{1/2} (\Phi_{00}, F'^* F' \Phi_{00})^{1/2} \\
&\quad = 2(\Phi_{11}, \Phi_{11})^{1/2} (\Phi_{00}, F'^* F' \Phi_{00})^{1/2}.
\end{aligned}$$

Inserting this into the identity above we finally obtain

$$\begin{aligned}
(\Psi, F^* F \Psi) \leq\ & (\Phi_{00}, F'^* F' \Phi_{00}) + (\Phi_{11}, F'^* F' \Phi_{11}) \\
& + 2\lambda_1^2 (\Phi_{11}, \Phi_{11}) + 2\sqrt{2}\lambda_1 (\Phi_{11}, \Phi_{11})^{1/2} (\Phi_{00}, F'^* F' \Phi_{00})^{1/2}. \quad (36)
\end{aligned}$$

Since $\Phi_{00} \in \bigwedge^N \mathfrak{h}'$, where $\mathfrak{h}'$ =span$\{u_3, \ldots, u_M\}$ and $F'$ only contains $a_3, \ldots, a_M$ we infer from the induction hypothesis that

$$(\Phi_{00}, F'^* F' \Phi_{00}) \leq (1 - \lambda_1^2) \|\Phi_{00}\|^2 \frac{N(M-N)}{M-2} = (1 - \lambda_1^2)(1 - \|\Phi_{11}\|^2) \frac{N(M-N)}{M-2}$$

Likewise since $\Phi_{11} = u_1 \wedge u_2 \wedge \Phi'$, with $\Phi' \in \bigwedge^{N-2} \mathfrak{h}'$ we get

$$(\Phi_{11}, F'^* F' \Phi_{11}) \leq (1 - \lambda_1^2) \|\Phi_{11}\|^2 \frac{(N-2)(M-N+2)}{M-2}.$$

If we denote by $Y = \|\Phi_{11}\|$ we have $0 \leq Y \leq 1$. We conclude from (36) that $(\Psi, F^* F \Psi) \leq \mathcal{G}(\lambda, Y)$ where

$$\begin{aligned}
\mathcal{G}(\lambda, Y) =\ & (1 - \lambda_1^2)(1 - Y^2) \frac{N(M-N)}{M-2} \\
& + (1 - \lambda_1^2) Y^2 \frac{(N-2)(M-N+2)}{M-2} + 2\lambda_1^2 Y^2 \\
& + 2\sqrt{2}\lambda_1 Y (1 - \lambda_1^2)^{1/2} (1 - Y^2)^{1/2} \left( \frac{N(M-N)}{M-2} \right)^{1/2}. \quad (37)
\end{aligned}$$

One may now analyze (see Appendix D for details) the function $\mathcal{G}(\lambda, Y)$ and show that for $0 \leq \lambda \leq 1$ and $0 \leq Y \leq 1$ its maximum is attained for

$$\lambda_1 = (2/M)^{1/2}, \quad Y = (N/M)^{1/2}. \quad (38)$$

where the maximal value is $\frac{N(M-N+2)}{N}$. $\square$

It follows from the proof above that the upper bound in Theorem 8.12 is optimal and one may go through the proof to find the $\Psi$ that optimizes the bound. In the next example we directly construct a $\Psi$ that achieves the bound in Theorem 8.12.

*EXAMPLE* 8.15 (A 2-particle density matrix with maximal eigenvalue). Our goal in this example is to show that the bound in the previous example is, in fact, optimal. We will explicitly write down a state $\Psi_N \in \bigwedge^N \mathfrak{h}$, where $\dim \mathfrak{h} = M$ such that the 2-particle density matrix $\Gamma^{(2)}_{\Psi_N}$ has eigenvalue $\frac{N(M-N+2)}{M}$, i.e., the largest possible. We will assume that $M = 2m$ and $N = 2n$ where $m$ and $n$ are positive integers. Let $u_1, \ldots, u_M$ be an orthonormal basis for $\mathfrak{h}$. Let $a_i = a_-(u_i)$. Hence $a_i^* = a_-^*(u_i)$. We define first a vector that does not have a fixed particle number

$$\Psi = c_0 \prod_{j=1}^{m} (1 + a_{2j-1}^* a_{2j}^*)|0\rangle. \tag{39}$$

Here $c_0$ is a positive normalization constant. We choose $\Psi_N$ to be a normalized vector in $\bigwedge^N \mathfrak{h}$ proportional (by a positive constant) to the projection of $\Psi$ onto $\bigwedge^N \mathfrak{h}$. We have

$$\Psi_N = \binom{m}{n}^{-1/2} \sum_{1 \le i_1 < \ldots < i_n \le m} \prod_{k=1}^{n} a_{2i_k-1}^* a_{2i_k}^* |0\rangle.$$

We claim that

$$f = \sum_{i=1}^{m} m^{-1/2} u_{2i-1} \wedge u_{2i}$$

is an eigenfunction of $\Gamma^{(2)}_{\Psi_N}$ with the largest possible eigenvalue.

**PROBLEM 8.16.** *Show that the above vector $f$ is normalized.*

Let

$$F = \sum_{i=1}^{m} \sqrt{2} m^{-1/2} a_{2i-1} a_{2i}.$$

Then as in (34) we have

$$(f, \Gamma^{(2)}_{\Psi_N} f) = (\Psi_N, F^* F \Psi_N).$$

**PROBLEM 8.17.** *Show (combinatorically) that* $(\Psi_N, F^* F \Psi_N) = \frac{N(M-N+2)}{M}$.

It follows from the previous problem that $(f, \Gamma^{(2)}_{\Psi_N} f)$ has the largest possible value among normalized $f$. It follows as in Problem 2.5 (used on $-\Gamma^{(2)}_{\Psi_N}$) that $f$ must be an eigenvector of $\Gamma^{(2)}_{\Psi_N}$ with eigenvalue $\frac{N(M-N+2)}{M}$.

The state in (39) as well as the Slater determinant states in Problem 1.24 and 8.5 are special cases of what are called *quasi-free* states. We will study these states in more detail in Section 10.

## 8.2 Generalized one-particle density matrix

If $\Psi \in \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$ does not have a fixed particle number it is also important to know $(\Psi, a_\pm(f)a_\pm(g)\Psi)$ and $(\Psi, a^*_\pm(f)a^*_\pm(g)\Psi)$. We will therefore consider a generalization of the one-particle density matrix.

**DEFINITION 8.18** (Generalized one-particle density matrix)**.** If $\Psi \in \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$ is a normalized vector with finite particle expectation we define the corresponding generalized one-particle density matrix to be the positive semi-definite operator $\Gamma_\Psi$ defined on $\mathfrak{h} \oplus \mathfrak{h}^*$ by

Correction since August 30, 09: Finite particle expectation added

$$(f_1 \oplus Jg_1, \Gamma_\Psi f_2 \oplus Jg_2)_{\mathfrak{h}\oplus\mathfrak{h}^*} = (\Psi, (a^*_\pm(f_2) + a_\pm(g_2))(a_\pm(f_1) + a^*_\pm(g_1))\Psi)_{\mathcal{F}^{\mathrm{B,F}}}.$$

Here as usual $J : \mathfrak{h} \to \mathfrak{h}^*$ is the conjugate linear map such that $Jg(f) = (g, f)$.

**PROBLEM 8.19.** *Show that $\Gamma_\Psi$ as defined above is indeed linear.*

**PROBLEM 8.20.** *Show that for fermions $0 \leq \Gamma_\Psi \leq I_{\mathfrak{h}\oplus\mathfrak{h}^*}$ and for bosons $\Gamma_\Psi \geq 0$, $\Gamma_\Psi \geq -\mathcal{S}$. (Compare Theorem 8.4).*

Correction since August 30, 09: Bosonic case added

We may write $\Gamma_\Psi$ in block matrix form corresponding to the direct sum decomposition $\mathfrak{h} \oplus \mathfrak{h}^*$

$$\Gamma_\Psi = \begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ \alpha^*_\Psi & 1 \pm J\gamma_\Psi J^* \end{pmatrix}. \tag{40}$$

Here $+$ is for bosons and $-$ is for fermions. The map $\gamma_\Psi : \mathfrak{h} \to \mathfrak{h}$ is the usual one-particle density matrix and $\alpha_\Psi : \mathfrak{h}^* \to \mathfrak{h}$ is the linear map given by

$$(f, \alpha_\Psi Jg) = (\Psi, a_\pm(g)a_\pm(f)\Psi). \tag{41}$$

The adjoint $J^*$ of the conjugate linear map $J$, which is, in fact, also the inverse $J^* = J^{-1}$, is discussed in Appendix E. The fact that the lower right corner of the matrix has the form given follows from the canonical commutation or anti-commutation relations in Problem 7.4

$$\begin{aligned}(\Psi, a_\pm(g_2)a^*_\pm(g_1)\Psi) &= (g_2, g_1) \pm (\Psi, a^*_\pm(g_1)a_\pm(g_2)\Psi) = (g_2, g_1) \pm (g_2, \gamma_\Psi g_1) \\ &= (Jg_1, Jg_2) \pm (Jg_1, J\gamma_\Psi J^* Jg_2) = (Jg_1, (1 \pm J\gamma_\Psi J^*)Jg_2).\end{aligned}$$

The linear map $\alpha_\Psi$ has the property

$$\alpha^*_\Psi = \pm J\alpha_\Psi J. \tag{42}$$

In fact, from the definition (41) we have

$$(\alpha^*_\Psi f, Jg) = (f, \alpha_\Psi Jg) = \pm(g, \alpha_\Psi Jf) = \pm(J\alpha_\Psi Jf, Jg).$$

Thus we may also write the generalized one-particle density matrix as

$$\Gamma_\Psi = \begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ \pm J\alpha_\Psi J & 1 \pm J\gamma_\Psi J^* \end{pmatrix}, \tag{43}$$

where $+$ is for bosons and $-$ is for fermions.

It will also be convenient to introduce the generalized annihilation and creation operators

$$A_\pm(f \oplus Jg) = a_\pm(f) + a^*_\pm(g) \tag{44}$$

$$A^*_\pm(f \oplus Jg) = a^*_\pm(f) + a_\pm(g). \tag{45}$$

Note that $A_\pm$ is a conjugate linear map from $\mathfrak{h} \oplus \mathfrak{h}^*$ to operators on $\mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$ and $A^*_\pm$ is a linear map. We have the relation

$$A^*_\pm(F) = A_\pm(\mathcal{J}F) \quad \text{where } \mathcal{J} = \begin{pmatrix} 0 & J^* \\ J & 0 \end{pmatrix} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*, \tag{46}$$

for all $F \in \mathfrak{h} \oplus \mathfrak{h}^*$. Using the generalized creation and annihilation operators we may express the canonical commutation relations as

$$[A_+(F_1), A^*_+(F_2)] = (F_1, \mathcal{S}F_2)_{\mathfrak{h}\oplus\mathfrak{h}^*}, \text{ where } \mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} : \mathfrak{h}\oplus\mathfrak{h}^* \to \mathfrak{h}\oplus\mathfrak{h}^* \tag{47}$$

and the canonical anti-commutation relations as

$$\{A_-(F_1), A^*_-(F_2)\} = (F_1, F_2)_{\mathfrak{h}\oplus\mathfrak{h}^*}. \tag{48}$$

We warn the reader that in general

$$[A_+(F_1), A_+(F_2)] \neq 0, \quad \{A_-(F_1), A_-(F_2)\} \neq 0.$$

In terms of the generalized creation and annihilation operators the generalized one-particle density matrix satisfies

$$(F_1, \Gamma_\Psi F_2)_{\mathfrak{h}\oplus\mathfrak{h}^*} = (\Psi, A_\pm^*(F_2)A_\pm(F_1)\Psi), \tag{49}$$

for all $F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}^*$.

Correction since August 30, 09: $A_\pm(F_2)^* \to A_\pm^*(F_2)$.

# 9 Bogolubov transformations

**DEFINITION 9.1** (Bogolubov maps)**.** A linear bounded isomorphism $\mathcal{V} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ is called a bosonic Bogolubov map if $A_+^*(\mathcal{V}F) = A_+(\mathcal{V}\mathcal{J}F)$ for all $F \in \mathfrak{h} \oplus \mathfrak{h}^*$ and

$$[A_+(\mathcal{V}F_1), A_+^*(\mathcal{V}F_2)] = (F_1, \mathcal{S}F_2), \tag{50}$$

for all $F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}^*$. It is called a fermionic Bogolubov map if $A_-^*(\mathcal{V}F) = A_-(\mathcal{V}\mathcal{J}F)$ for all $F \in \mathfrak{h} \oplus \mathfrak{h}^*$ and

$$\{A_-(\mathcal{V}F_1), A_-^*(\mathcal{V}F_2)\} = (F_1, F_2). \tag{51}$$

for all $F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}^*$.

This definition simply says that a Bogolubov map $\mathcal{V}$ is characterized by $F \mapsto A_\pm(\mathcal{V}F)$ having the same properties ((46) and (47) or (48)) as $F \mapsto A_\pm(F)$.

If $\mathcal{V}$ is a Bogolubov map then one often refers to the operator transformation $A_\pm(F) \to A_\pm(\mathcal{V}F)$ as a *Bogolubov or (Bogolubov-Valatin) transformation.*

Using (46) and (47) we may rewrite the conditions for being a bosonic Bogolubov map as

$$(\mathcal{V}F_1, \mathcal{S}\mathcal{V}F_2) = (F_1, \mathcal{S}F_2), \quad \text{and} \quad \mathcal{J}\mathcal{V}F = \mathcal{V}\mathcal{J}F$$

for all $F, F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}^*$. Likewise, using (46) and (48) we may rewrite the conditions for being a fermionic Bogolubov map as

$$(\mathcal{V}F_1, \mathcal{V}F_2) = (F_1, F_2), \quad \text{and} \quad \mathcal{J}\mathcal{V}F = \mathcal{V}\mathcal{J}F$$

for all $F, F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}^*$.

Since we are assuming that $\mathcal{V}$ is invertible we see that

$$\mathcal{V}^{-1} = \mathcal{S}\mathcal{V}^*\mathcal{S} \tag{52}$$

in the bosonic case and

$$\mathcal{V}^{-1} = \mathcal{V}^* \tag{53}$$

in the fermionic case.

Thus we immediately conclude the following reformulation of the definition of Bogolubov maps.

Correction since June 24: Theorem reformulated

**THEOREM 9.2** (Bogolubov maps)**.** *A linear map $\mathcal{V} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ is a bosonic Bogolubov map if and only if*

$$\mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{S}, \quad \mathcal{V}\mathcal{S}\mathcal{V}^* = \mathcal{S}, \quad \mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V}. \tag{54}$$

*It is a fermionic Bogolubov map if and only if*

$$\mathcal{V}^*\mathcal{V} = I_{\mathfrak{h}\oplus\mathfrak{h}^*}, \quad \mathcal{V}\mathcal{V}^* = I_{\mathfrak{h}\oplus\mathfrak{h}^*}, \quad \mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V}. \tag{55}$$

*A fermionic Bogolubov map is, in particular, unitary.*

**PROBLEM 9.3.** *Show that the Bogolubov maps form a subgroup of the group of isomorphism of $\mathfrak{h} \oplus \mathfrak{h}^*$.*

We may write a Bogolubov map as a block matrix

$$\mathcal{V} = \begin{pmatrix} U & J^*VJ^* \\ V & JUJ^* \end{pmatrix}, \tag{56}$$

where $U : \mathfrak{h} \to \mathfrak{h}$, $V : \mathfrak{h} \to \mathfrak{h}^*$. That a Bogolubov map must have the special matrix form (56) follows immediately from the condition $\mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V}$. In order for the matrix (56) to be a Bogolubov map we see from (54) and (55) that $U$ and $V$ must also satisfy the conditions

$$U^*U = 1 \pm V^*V, \quad JV^*JU = \pm JU^*J^*V \tag{57}$$

where $+$ is for bosons and $-$ is for fermions. We also get from (54) and (55) that

Correction since August 30, 09: $\mp \to \pm$

$$UU^* = 1 \pm J^* V V^* J \tag{58}$$

again with $-$ for bosons and $+$ for fermions.

We shall next show that the Bogolubov transformations $A_\pm(F) \mapsto A_\pm(\mathcal{V}F)$ may be implemented by a unitary map on the Fock spaces $\mathcal{F}^{\mathrm{B,F}}$. We will need the following result.

**PROBLEM 9.4.** *Assume that $u_1, u_2 \ldots$ are orthonormal vectors in $\mathfrak{h}$. Consider for some positive integers, $M, n_1, \ldots, n_M$ the vector*

$$a_\pm^*(u_M)^{n_M} \cdots a_\pm^*(u_1)^{n_1}|0\rangle \in \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h}).$$

*Show that in the bosonic case the vector has norm $(n_1! \cdots n_M!)^{1/2}$ for all non-negative integers $n_1, \ldots, n_M$. Show that in the fermionic case the vector vanishes unless $n_1, \ldots, n_M$ are all either 1 or 0 and in this cases the vector is normalized.*

Correction since August 30, 09: "either 1" → "either 1 or 0".

**THEOREM 9.5** (Unitary Bogolubov implementation)**.** *If $\mathcal{V} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ is a Bogolubov map (either fermionic or bosonic) of the form (56) then there exists a unitary transformation*

$$\mathbb{U}_\mathcal{V} : \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h}) \to \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$$

*such that*

$$\mathbb{U}_\mathcal{V} A_\pm(F) \mathbb{U}_\mathcal{V}^* = A_\pm(\mathcal{V}F)$$

*for all $F \in \mathfrak{h} \oplus \mathfrak{h}^*$ if and only if $V^*V$ is trace class. This trace class condition is referred to as the Shale-Stinespring condition.*

*Proof.* The proof is somewhat complicated and we will give a sketchy presentation leaving details to the interested reader.

We assume first $V^*V$ is trace class and will construct the unitary $\mathbb{U}_\mathcal{V}$. Let $u_1, u_2, \ldots$ be an orthonormal basis for $\mathfrak{h}$. We have an orthonormal basis for $\mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$ given by (see Problem 9.4)

$$|n_{i_1}, \ldots, n_{i_M}\rangle = (n_{i_1}! \cdots n_{i_M}!)^{-1/2} a_\pm^*(u_{i_M})^{n_{i_M}} \cdots a_\pm^*(u_{i_1})^{n_{i_1}}|0\rangle,$$

where $M = 1, 2, \ldots$, $1 \le i_1 < i_2 < \ldots < i_M$ run over the positive integers. For bosons $n_1, \ldots, n_M$ run over positive integers and for fermions they are all 1.

We will construct the unitary $\mathbb{U}_{\mathcal{V}}$ by constructing the orthonormal basis

$$|n_{i_1}, \ldots, n_{i_M}\rangle_{\mathcal{V}} = \mathbb{U}_{\mathcal{V}}|n_{i_1}, \ldots, n_{i_M}\rangle.$$

The main difficulty is to construct the vacuum $|0\rangle_{\mathcal{V}} = \mathbb{U}_{\mathcal{V}}|0\rangle$. Recall that $A_\pm(u \oplus 0) = a_\pm(u)$ are the annihilation operators and that $A_\pm(0 \oplus Ju)) = a^*_\pm(u)$ are the creation operators. Thus if $\mathbb{U}_{\mathcal{V}}$ exists the new vacuum must be characterized by

$$A_\pm(\mathcal{V}(u_i \oplus 0))|0\rangle_{\mathcal{V}} = \mathbb{U}_{\mathcal{V}} A_\pm(u_i \oplus 0)\mathbb{U}^*_{\mathcal{V}}\mathbb{U}_{\mathcal{V}}|0\rangle = \mathbb{U}_{\mathcal{V}} A_\pm(u_i \oplus 0)|0\rangle = 0,$$

for all $i = 1, 2,$ i.e., by being annihilated by all the new annihilation operators $A_\pm(\mathcal{V}(u_i \oplus 0))$. We shall construct the new vacuum below.

Having constructed the new vacuum $|0\rangle_{\mathcal{V}}$ the rest of the proof is fairly easy. We must have

$$\begin{aligned} &|n_{i_1}, \ldots, n_{i_M}\rangle_{\mathcal{V}} = \mathbb{U}_{\mathcal{V}}|n_{i_1}, \ldots, n_{i_M}\rangle \\ &= (n_{i_1}! \cdots n_{i_M}!)^{-1/2}\mathbb{U}_{\mathcal{V}} A_\pm(0 \oplus Ju_{i_M})^{n_{i_M}} \cdots A_\pm(0 \oplus Ju_{i_1})^{n_{i_1}}\mathbb{U}^*_{\mathcal{V}}\mathbb{U}_{\mathcal{V}}|0\rangle \\ &= (n_{i_1}! \cdots n_{i_M}!)^{-1/2} A_\pm(\mathcal{V}(0 \oplus Ju_{i_M}))^{n_{i_M}} \cdots A_\pm(\mathcal{V}(0 \oplus Ju_{i_1}))^{n_{i_1}}|0\rangle_{\mathcal{V}}. \end{aligned}$$

It follows from the fact, that the new creation operators and the new annihilation operators satisfy the canonical commutation or anti-commutation relations that the vectors $|n_{i_1}, \ldots, n_{i_M}\rangle_{\mathcal{V}}$ will form an orthonormal family. All we have to show is that they form a basis. To do this we simply revert the construction and construct the old basis vectors $|n_{i_1}, \ldots, n_{i_M}\rangle$ from the new $|n_{i_1}, \ldots, n_{i_M}\rangle_{\mathcal{V}}$ by simply interchanging the roles of the old and the new basis vectors and of $\mathcal{V}$ and $\mathcal{V}^{-1}$. Doing this we will be able to express the old basis vectors as (possibly infinite) linear combinations of the new basis vectors, thus showing that the new vectors indeed span the whole space. We will leave this reversion of the construction to the interested reader.

Correction since August 30, 09: old basis vectors $|n_{i_1}, \ldots, n_{i_M}\rangle_{\mathcal{V}} \to |n_{i_1}, \ldots, n_{i_M}\rangle$

It remains to construct the new vacuum. We first choose a particularly useful orthonormal basis of $\mathfrak{h}$. We use the notation of (56). Note that the linear Hermitian matrix $U^*U$ commutes with the conjugate linear map $C = U^*J^*V$. In fact, from (58) and (57) we have

$$\begin{aligned} U^*UC = U^*UU^*J^*V &= U^*(1 \pm J^*VV^*J)J^*V = U^*J^*V \pm U^*J^*VV^*V \\ &= U^*J^*V + U^*J^*V(U^*U - 1) = CU^*U. \end{aligned}$$

Since $V^*V$ is trace class it has an orthonormal basis of eigenvectors. The relation (57) shows that this is also an eigenbasis for $U^*U$. It follows from (58) that

$$C^*C = V^*JUU^*JV = V^*(1 \pm VV^*)V = V^*V \pm (V^*V)^2$$

and thus $C^*C$ is trace class.

Since the eigenvalues of $U^*U$ are real it follows that $C$ maps each eigenspace of $U^*U$ into itself. Indeed, if $v \in \mathfrak{h}$ satisfies $U^*Uv = \lambda v$ for $\lambda \in \mathbb{R}$ we have $U^*UCv = CU^*Uv = \lambda Cv$.

From (57) we see that the map $C$ is a conjugate Hermitian map for bosons and a conjugate anti-Hermitian map for fermions. We may therefore find an orthonormal basis for each eigenspace of $U^*U$ according to Theorem E.2.

This means that we can find an orthonormal basis $u_1, u_2 \ldots$ of $\mathfrak{h}$ consisting of eigenvectors of $U^*U$, denoting the eigenvalues $\mu_1^2, \mu_2^2 \ldots$ (assuming that $\mu_1, \ldots \geq 0$), such that in the bosonic case they are also eigenvectors of $C$ with real eigenvalues $\lambda_1, \lambda_2 \ldots$, or in the fermionic case there are $I' \subset \mathbb{N}$ and $I'' = \mathbb{N} \backslash \{2i, 2i-1 | i \in I'\}$ satisfying

Correction since August 30, 09: Redefine $I'$ and $I''$.

$$Cu_{2i} = \lambda_i u_{2i-1},\ Cu_{2i-1} = -\lambda_i u_{2i}, \qquad i \in I'$$

where $\lambda_i > 0$ and

$$Cu_i = 0, \qquad i \in I''.$$

We have according to (56) the new annihilation operators

$$A_\pm(\mathcal{V}(u_i \oplus 0)) = A_\pm((Uu_i \oplus Vu_i)) = \mu_i a_\pm(f_i) + a_\pm^*(g_i), \tag{59}$$

where for $i = 1, 2 \ldots$ we have introduced $g_i = J^*Vu_i$ and

$$f_i = \begin{cases} \mu_i^{-1}Uu_i, & \text{if } \mu_i \neq 0 \\ 0, & \text{if } \mu_i = 0 \end{cases}.$$

The new creation operators are (of course) the adjoints of the annihilation operators, but this indeed agrees with (56) since

$$A_\pm(\mathcal{V}(0 \oplus Ju_i)) = A_\pm((J^*Vu_i \oplus JUu_i) = a_\pm(g_i) + \mu_i a_\pm^*(f_i).$$

In the bosonic case it follows from (57) that $\mu_i \geq 1$, thus in this case we have $(f_i, f_j) = \mu_i^{-2}(u_i, U^*Uu_j) = \delta_{ij}$ and the $f_i$ are orthonormal. Since $U$ is

Correction since June 22 injective $\to$ surjective a surjective map (since $U^*$ is invertible by (58)) the $f_i$ form an orthonormal basis for $\mathfrak{h}$. Moreover, $(f_i, g_j) = \mu_i^{-1}(Uu_i, J^*Vu_j) = \mu_i^{-1}(u_i, Cu_j) = \lambda_i/\mu_i\delta_{ij}$. Let $\nu_i = \lambda_i/\mu_i$. Thus $g_i = \nu_i f_i$. From (57)

$$\nu_i^2 = \frac{\lambda_i^2}{\mu_i^2} = (g_i, g_i) = (u_i, V^*Vu_i) = (u_i, (U^*U - 1)u_i) = \mu_i^2 - 1.$$

We conclude that in the bosonic case there is an orthonormal basis $f_1, f_2 \ldots,$ for $\mathfrak{h}$ and numbers $\mu_i \geq 1, \nu_i \in \mathbb{R}$, for $i = 1, \ldots$ such that the new bosonic annihilation operators are

$$A_+(\mathcal{V}(u_i \oplus 0)) = \mu_i a_+(f_i) + \nu_i a_+^*(f_i), \quad \mu_i^2 - \nu_i^2 = 1 \tag{60}$$

for $i = 1, 2 \ldots$.

We can now in the bosonic case find the new vacuum vector $|0\rangle_{\mathcal{V}}$ characterized by being annihilated by all the new annihilation operators. Indeed,

$$\begin{aligned}
|0\rangle_{\mathcal{V}} &= \lim_{M\to\infty} \prod_{j=1}^{M} (1 - (\nu_j/\mu_j)^2)^{1/4} \sum_{n=0}^{\infty} \left(\frac{-\nu_j}{2\mu_j}\right)^n \frac{a_+^*(f_j)^{2n}}{n!} |0\rangle \\
&= \prod_{j=1} (1 - (\nu_j/\mu_j)^2)^{1/4} \sum_{n=0}^{\infty} \left(\frac{-\nu_j}{2\mu_j}\right)^n \frac{a_+^*(f_j)^{2n}}{n!} |0\rangle \\
&= \left(\prod_{j=1} (1 - (\nu_j/\mu_j)^2)^{1/4}\right) \exp\left[-\sum_{i=1} \frac{\nu_i}{2\mu_i} a_+^*(f_i)^2\right] |0\rangle. \qquad (61)
\end{aligned}$$

Here the exponential is really just a convenient way of writing the power series. The normalization factor follows from the Taylor series expansion

$$(1 - 4t^2)^{-1/2} = \sum_{n=0}^{\infty} \frac{t^{2n}(2n)!}{(n!)^2},$$

which gives for all $i$

$$\begin{aligned}
&(1 - (\nu_i/\mu_i)^2)^{1/2} \sum_{n=0}^{\infty} \frac{\langle 0|a_+(f_i)^{2n} a_+^*(f_i)^{2n}|0\rangle (\nu_i/2\mu_i)^{2n}}{(n!)^2} \\
&= (1 - (\nu_i/\mu_i)^2)^{1/2} \sum_{n=0}^{\infty} \frac{(2n)!(\nu_i/2\mu_i)^{2n}}{(n!)^2} = 1.
\end{aligned}$$

Using that $V^*V$ is trace class and hence that $\sum_{i=1} \nu_i^2 < \infty$ we shall now see that the limit $M \to \infty$ above exists. Define

$$\Psi_M = \prod_{j=1}^{M} (1 - (\nu_j/\mu_j)^2)^{1/4} \exp\left[-\sum_{i=1}^{M} \frac{\nu_i}{2\mu_i} a_+^*(f_i)^2\right] |0\rangle.$$

We have

$$\|\Psi_N - \Psi_M\|^2 = 2 - 2\prod_{j=M+1}^{N}(1-(\nu_j/\mu_j)^2)^{1/4} \to 0$$

as $M \to \infty$ uniformly in $N > M$. Thus $\Psi_M$ is Cauchy sequence.

Since $f_i$ is orthogonal to $f_j$ for $i \neq j$ the creation and annihilation operators $a_+(f_i), a_+^*(f_i)$ commute with $a_+(f_j), a_+^*(f_j)$ if $i \neq j$. Using this it is a fairly straightforward calculation to see that

$$(\mu_i a_+(f_i) + \nu_i a_+^*(f_i))|0\rangle_{\mathcal{V}} = 0$$

for all $i = 1, \ldots$, which is what we wanted to prove.

We turn to the fermionic case. Our goal is to show that if we define

$$\eta_i = \begin{cases} f_i, & \text{if } \mu_i \neq 0 \\ g_i, & \text{if } \mu_i = 0 \end{cases} \tag{62}$$

then $\eta_1, \eta_2 \ldots$ is an orthonormal basis for $\mathfrak{h}$. We claim moreover that the new annihilation operators may be written

Correction since June 24: $i \to 2i$ several places

Correction since August 30, 09: undo correction June 24; $A_-(\mathcal{V}(\eta_j \oplus 0)) \to A_-(\mathcal{V}(u_j \oplus 0))$; adding the possibility of $\alpha_i$

$$\begin{aligned} A_-(\mathcal{V}(u_{2i-1}\oplus 0)) &= \alpha_i a_-(\eta_{2i-1}) - \beta_i a_-^*(\eta_{2i}), \quad i \in I' && (63)\\ A_-(\mathcal{V}(u_{2i}\oplus 0)) &= \alpha_i a_-(\eta_{2i}) + \beta_i a_-^*(\eta_{2i-1}), \quad i \in I' && (64)\\ A_-(\mathcal{V}(u_i\oplus 0)) &= a_-^*(\eta_i), \quad i \in I_k'' && (65)\\ A_-(\mathcal{V}(u_i\oplus 0)) &= a_-(\eta_i), \quad i \in I'' \setminus I_k'', && (66) \end{aligned}$$

where $k$ is a non-negative integer and $I_k''$ refers to the first $k$ elements of $I''$, $\alpha_i = \mu_{2i} > 0$, $\beta_i \geq 0$ and $\alpha_i^2 + \beta_i^2 = 1$, for $i \in I'$.

Before proving this we observe that it is easy to see from this representation that the following normalized vector is annihilated by all the operators in (63–65)

Correction since August 30, 09: $\beta_i \to -\beta_i$

$$\begin{aligned} |0\rangle_{\mathcal{V}} &= \left(\prod_{i\in I_k''} a_-^*(\eta_i)\right)\prod_{2i\in I'}(\alpha_i - \beta_i a_-^*(\eta_{2i})a_-^*(\eta_{2i-1}))|0\rangle \\ &= \left(\prod_{i\in I_k''} a_-^*(\eta_i)\right)\left(\prod_{2i\in I'}\alpha_i\right)\exp\left(-\sum_{2i\in I'}\frac{\beta_i}{\alpha_i}a_-^*(\eta_{2i})a_-^*(\eta_{2i-1})\right)|0\rangle. \end{aligned} \tag{67}$$

Again this vector should really be defined by a limiting procedure. Since $V^*V$ is trace class we have from (57) that $\sum_i(1-\mu_i^2) < \infty$ and thus $\prod_{i\in I'}\alpha_i^2 = \prod_{i\in I'}\mu_{2i}^2 > 0$. The limiting procedure is hence justified as in the bosonic case.

Correction since August 30, 09: Positivity of $\prod_{i\in I'}\alpha_i^2$ added.

To prove (63)–(65) we return to (59). We have as in the bosonic case $(f_i, f_j) = \mu_i^{-1}\mu_j^{-1}(Uu_i, Uu_j) = \delta_{ij}$ if $\mu_i, \mu_j \neq 0$. From (57) we have

$$(g_i, g_j) = (u_j, V^*Vu_i) = (u_j, (1-U^*U)u_i) = (1-\mu_i^2)\delta_{ij}.$$

Thus for all $i, j = 1, 2, \ldots$ with $i \neq j$, $g_i$ is orthogonal to $g_j$ and if $\mu_i = 0$ $g_i$ is normalized.

We now prove that

$$J^*V\,\mathrm{Ker}(U) = \mathrm{Ker}(U^*). \tag{68}$$

Correction since August 30, 09: Some small changes in this part of the proof

Indeed, if $g \in \mathrm{Ker}(U)$ then $g = V^*Vg$, and $J^*Vg \in \mathrm{Ker}(U^*)$ due to

$$UU^*J^*Vg = (1 - J^*VV^*J)J^*Vg = J^*V(1-V^*V)g = 0.$$

Similarly, if $g \in \mathrm{Ker}(U^*)$ then $g = J^*VV^*Jg \in J^*V\,\mathrm{Ker}(U)$ since

$$U^*UV^*Jg = (1-V^*V)V^*Jg = V^*J(1-J^*VV^*J)g = 0.$$

From (68) and

$$\mathrm{Span}\{\eta_i : \mu_i = 0\} = \mathrm{Ker}(U^*) = \mathrm{Ran}(U)^\perp = \mathrm{Span}\{\eta_i : \mu_i \neq 0\}^\perp,$$

we conclude that $\eta_1$, $\eta_2$,... form an orthonormal basis for $\mathfrak{h}$.

Now we give a deeper description for $\eta_i$ with respect to $i \in I'$ and $i \in I''$. We first consider $i \in I'$. Since $u_{2i} \notin \mathrm{Ker}(C) \supset \mathrm{Ker}(U)$, we have $Uu_{2i} \neq 0$ and hence $\mu_{2i} \neq 0$. Likewise $\mu_{2i-1} \neq 0$. Thus $\eta_{2i} = f_{2i}$ and $\eta_{2i-1} = f_{2i-1}$.

Moreover, for all j we have

$$(Uu_j, g_{2i}) = (Uu_j, J^*Vu_{2i}) = (u_j, Cu_{2i}) = \lambda_i\delta_{2i-1,j}. \tag{69}$$

Thus since $g_{2i}$ is orthogonal to all $\eta_j$ with $j \neq 2i-1$ we conclude that

$$g_{2i} = \lambda_i\mu_{2i-1}^{-1}\eta_{2i-1}. \tag{70}$$

and likewise

$$g_{2i-1} = -\lambda_i\mu_{2i}^{-1}\eta_{2i}. \tag{71}$$

From (70) we obtain

$$\lambda_i^2\mu_{2i-1}^{-2} = (g_{2i}, g_{2i}) = (V^*Vu_{2i}, u_{2i}) = ((1-U^*U)u_{2i}, u_{2i}) = 1 - \mu_{2i}^2$$

and likewise from (71) we get

$$\lambda_i^2 \mu_{2i}^{-2} = 1 - \mu_{2i-1}^2.$$

These two identities imply that $\mu_{2i} = \mu_{2i-1}$.

Then (63–64) follow from (70)–(71) with $\alpha_i = \mu_{2i} = \mu_{2i-1}$ and $\beta_i = \lambda_i \mu_{2i}^{-1} = \lambda_i \mu_{2i-1}^{-1}$.

For $i \in I''$ we have

$$0 = (u_i, C^* C u_i) = (u_i, U^* U(U^* U - 1) u_i) = \mu_i^2(\mu_i^2 - 1).$$

Thus we conclude that either $\mu_i = 1$ and hence $g_i = 0$, or $\mu_i = 0$ and hence $g_i = \eta_i$. In the former case we must have $A_-(\mathcal{V}(u_i \oplus 0)) = a_-(\eta_i)$ and in the latter case $A_-(\mathcal{V}(u_i \oplus 0)) = a_-^*(\eta_i)$. Since $V^* V$ is trace class the eigenvalue 1 has finite multiplicity. This means that the eigenvalue $\mu_i = 0$ for $U^* U$ has finite multiplicity $k$. We can assume that $I''$ has been ordered such that $\mu_i = 0$ occurs for the first $k$ i.

The necessity of the Shale-Stinespring condition is proved in Appendix F. □

In the rest of this chapter we shall see that for each normalized state $\Psi \in \mathcal{F}^{B,F}(\mathfrak{h})$ we may find a Bogolubov map $\mathcal{V}$ diagonalizing the 1-pdm of $\mathbb{U}_{\mathcal{V}}^* \Psi$.

**LEMMA 9.6.** *Assume that a Hermitian $\mathcal{A} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ satisfies*

Correction since August 30, 09: Lemma refomulated for infinite dimension

$$\mathcal{J}\mathcal{A}\mathcal{J} = \pm \mathcal{A} \quad \textit{(+ for bosons and − for fermions).} \tag{72}$$

*Assume moreover in the fermionic case that $\mathcal{A}$ admits an eigenbasis for $\mathfrak{h} \oplus \mathfrak{h}^*$, and assume in the bosonic case that $\mathcal{A}$ is positive definite and $\mathcal{S}\mathcal{A}$ admits an eigenbasis for $\mathfrak{h} \oplus \mathfrak{h}^*$. Then for any orthonormal basis $u_1, u_2, \ldots$ for $\mathfrak{h}$, there exists a bosonic (+) or fermionic (-) Bogolubov map $\mathcal{V}$ such that the operator $\mathcal{V}^* \mathcal{A} \mathcal{V}$ has eigenvectors of the form $\{u_n \oplus 0\} \cup \{0 \oplus J u_n\}$.*

Note that in general $\mathcal{V}$ need not admit a unitary implementation.

*Proof.* We will construct $\mathcal{V}$ by finding the vectors

$$v_{2n} = \mathcal{V}(u_n \oplus 0), \widetilde{v}_n = \mathcal{V}(0 \oplus J u_n).$$

We first consider the fermionic case. It is straightforward to check that $\mathcal{V}$ will satisfy the required properties if $\{v_n\} \cup \{\widetilde{v}_n\}$ form an orthonormal basis of eigenvectors of $\mathcal{A}$ such that for all $n = 1, 2, \ldots$

$$\widetilde{v}_n = \mathcal{J} v_j.$$

Let $v_1$ be a normalized eigenvector of $\mathcal{A}$ with eigenvalue $\lambda_1$. Define $\widetilde{v}_1 = \mathcal{J} v_1$. Then $\widetilde{v}_1$ is a normalized vector and from (72) we have that

$$\mathcal{A}\widetilde{v}_1 = -\mathcal{J}\mathcal{A}v_1 = -\mathcal{J}\lambda_1 v_1 = -\lambda_1 \widetilde{v}_1,$$

where we have used that $\lambda_1$ is real.

Thus $\widetilde{v}_1$ is an eigenvector of $\mathcal{A}$. Moreover, if $\lambda_1 \neq 0$ it follows that the eigenvalues $\lambda_1$ and $-\lambda_1$ are different and hence that $\widetilde{v}_1$ is orthogonal to $v_1$. We may then restrict $\mathcal{A}$ to the orthogonal complement of the space spanned by $v_1$ and $\widetilde{v}_1$ and continue the process in this way we will find an orthonormal family of vectors of the desired form. They will however not necessarily form a basis since we still have to consider the kernel of $\mathcal{A}$.

It follows from (72) that $\mathcal{J}$ maps the kernel of $\mathcal{A}$ to itself. We may then using Theorem E.2 to find an orthonormal basis for the kernel consisting of eigenvectors of $\mathcal{J}$ with non-negative eigenvalues. Since, $\mathcal{J}^2 = I$ the eigenvalues are 1. If $w_1$ and $w_2$ are two basis vectors the vectors $v_\pm = \frac{w_1 \pm i w_2}{\sqrt{2}}$ are orthonormal and they satisfy $\mathcal{J} v_\pm = v_\mp$. By pairing the basis vectors for the kernel of $\mathcal{A}$ in this manner we find a basis of the desired form. This completes the proof in the fermionic case.

Correction since August 30, 09: Theorem E.2 formulated for non-compact operators.

Correction since August 30, 09: $w_1 \pm i w_2 \to \frac{w_1 \pm i w_2}{\sqrt{2}}$.

We turn to the bosonic case. It is again straightforward to check that we have to show the existence of a basis $\{v_i\} \cup \{\widetilde{v}_i\}$ for $\mathfrak{h} \oplus \mathfrak{h}^*$ with the following properties

1. $(v_i, \mathcal{S} v_j) = \delta_{ij}, (\widetilde{v}_i, \mathcal{S}\widetilde{v}_j) = -\delta_{ij}$ and $(v_i, \mathcal{S}\widetilde{v}_j) = 0$ for all $i, j = 1, 2, \ldots$

2. $v_j, \widetilde{v}_j$ are eigenvectors of $\mathcal{S}\mathcal{A}$ for all $j = 1, 2, \ldots$

3. $\mathcal{J} v_j = \widetilde{v}_j$ for all $j = 1, 2, \ldots$

Note that item 2 is not an eigenvalue problem for $\mathcal{A}$, but for $\mathcal{S}\mathcal{A}$, which is not Hermitian. Still it can be analyzed in much the same way as the eigenvalue problem for a Hermitian matrix.

Let $v_1$ be a normalized eigenvector of $\mathcal{SA}$ with eigenvalue $\lambda_1$. We have from $\mathcal{A}v_1 = \lambda_1\mathcal{S}v_1$ that

$$(v_1, \mathcal{A}v_1) = \lambda_1(v_1, \mathcal{S}v_1).$$

Since $\mathcal{A}$ is possitive definite and $\mathcal{S}$ is Hermitian, $\lambda_1$ must be real and non-zero, moreover we can assume that $v_1$ has been normalized in such a way that $(v_1, \mathcal{S}v_1) = \pm 1$.

Correction since August 30, 09: $(v_1, \mathcal{S}v_1) = 1 \to \pm 1$

Define $\widetilde{v}_1 = \mathcal{J}v_1$ then using (72) we have that

$$\mathcal{SA}\widetilde{v}_1 = \mathcal{SJA}v_1 = -\mathcal{JSA}v_1 = -\mathcal{J}\lambda_1 v_1 = -\lambda_1 v_{M+1},$$

where we have used that $\lambda_1$ is real and that $\mathcal{JS} = -\mathcal{SJ}$. Thus $\widetilde{v}_1$ satisfies 2 with $\widetilde{\lambda}_1 = -\lambda_1$.

Since $\lambda_1 \neq 0$ then $\widetilde{\lambda}_1 \neq \lambda_1$ and we conclude from

$$\widetilde{\lambda}_1(v_1, \mathcal{S}\widetilde{v}_1) = (v_1, \mathcal{A}\widetilde{\lambda}_1) = (\mathcal{A}v_1, \widetilde{v}_1) = \lambda_1(v_1, \mathcal{S}\widetilde{v}_1)$$

that $(v_1, \mathcal{S}\widetilde{v}_1) = 0$. Since we also have

$$(\widetilde{v}_1, \mathcal{S}\widetilde{v}_1) = (\mathcal{J}v_1, \mathcal{SJ}v_1) = (\mathcal{J}v_1, -\mathcal{JS}v_1) = -(\mathcal{S}v_1, v_1) = -(v_1, \mathcal{S}v_1),$$

by interchanging $v_1$ and $\widetilde{v}_1$ if necessary, we can assume that $(v_1, \mathcal{S}v_1) = 1$ and $(\widetilde{v}_1, \mathcal{S}\widetilde{v}_1) = -1$. Now we see that $v_1$ and $\widetilde{v}_1$ satisfy item 1.

We next show that $\mathcal{SA}$ maps the subspace

$$X = \{w \mid (v_1, \mathcal{S}w) = (\widetilde{v}_1, \mathcal{S}w) = 0\}$$

into itself. Indeed, if $w$ is in this space we have

$$(v_1, \mathcal{SSA}w) = (v_1, \mathcal{A}w) = (\mathcal{A}v_1, w) = \lambda_1(\mathcal{S}v_1, w) = 0$$

and likewise for $\widetilde{v}_1$. We then can restrict $\mathcal{SA}$ on $X$ and we can continue the argument by induction. The fact that $\mathcal{SA}$ admits an eigenbasis on $X$ is an exercise left for the reader. $\square$

Correction since August 30, 09: Problem added

**PROBLEM 9.7** (Compare to E.3)**.** *Let $\mathfrak{h}$ be a Hilbert space, $V$ be a closed subspace of $\mathfrak{h} \oplus \mathfrak{h}^*$ and*

$$W = \{w \in \mathfrak{h} \oplus \mathfrak{h}^* | (v, \mathcal{S}w) = 0 \text{ for all } v \in V\}.$$

*Prove that*

$$W = \mathcal{S}(V^{\perp}) = (\mathcal{S}V)^{\perp} \quad \text{and} \quad \mathfrak{h} \oplus \mathfrak{h}^* = V \oplus W.$$

*Let $f$ be a linear operator on $\mathfrak{h} \oplus \mathfrak{h}^*$ which leaves invariant $V$ and $W$. Show that if $f$ has an eigenvector $u \in \mathfrak{h} \oplus \mathfrak{h}^* \backslash V$ then $f$ also has an eigenvector $v \in W$ such that $u \in \mathrm{Span}(V \cup \{v\})$.*

**PROBLEM 9.8.** *Consider $\mathfrak{h} = \mathbb{C}$. The map $J$ may be identified with complex conjugation. We use the basis $1 \oplus 0$ and $0 \oplus 1$ for $\mathfrak{h} \oplus \mathfrak{h}^*$. In this basis we consider*

$$\mathcal{A} = \begin{pmatrix} 1 & a \\ a & 1 \end{pmatrix},$$

*for $0 < a < 1$. Show that we have a bosonic Bogolubov map defined by*

Correction since June 24: b→B

$$\mathcal{V} = \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{a}{\sqrt{\sqrt{1-a^2}-1+a^2}} & \frac{\left(\sqrt{1-a^2}-1\right)}{\sqrt{\sqrt{1-a^2}-1+a^2}} \\ \frac{\left(\sqrt{1-a^2}-1\right)}{\sqrt{\sqrt{1-a^2}-1+a^2}} & \frac{a}{\sqrt{\sqrt{1-a^2}-1+a^2}} \end{pmatrix}$$

*which diagonalizes $\mathcal{A}$ and determine the diagonal elements. What happens when $a = 1$?*

Correction since August 30, 09: Theorem refomulated for infinite dimension

Correction since August 30, 09: Finite particle expectation added

**THEOREM 9.9** (Diagonalizing generalized 1pdm)**.** *Let $\Psi \in \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$ be a normalized vector with finite particle expectation and $u_1, u_2, \ldots$ be an orthonormal basis for $\mathfrak{h}$. Then there exists a Bogolubov map $\mathcal{V} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$, such that the corresponding unitary map $\mathbb{U}_{\mathcal{V}}$ has the property that the generalized 1-particle density matrix of $\mathbb{U}_{\mathcal{V}}^*\Psi$ is a diagonal matrix in the orthonormal basis $\{u_n \oplus 0\} \cup \{0 \oplus Ju_n\}$ for $\mathfrak{h} \oplus \mathfrak{h}^*$.*

*Proof.* Using (49) it is straightforward to check that

$$\Gamma_{\mathbb{U}_{\mathcal{V}}^*\Psi} = \mathcal{V}^*\Gamma_\Psi\mathcal{V}.$$

We observe that (43) may be reformulated as

$$\mathcal{J}(\Gamma_\Psi \pm \tfrac{1}{2}\mathcal{S}_\pm)\mathcal{J} = \Gamma_\Psi + \tfrac{1}{2}\mathcal{S}_\pm \tag{73}$$

where (+) for boson with $\mathcal{S}_+ = \mathcal{S}$ and (-) for fermion with $\mathcal{S}_- = I$. To apply Lemma 9.6, this observation suggests us to introduce the operators

$$\mathcal{A}_\pm = \Gamma_\Psi \pm \tfrac{1}{2}\mathcal{S}_\pm = \begin{pmatrix} \gamma \pm \frac{1}{2} & \alpha \\ \alpha^* & \pm J\gamma J^* + \frac{1}{2} \end{pmatrix}$$

where $\gamma$ and $\alpha$ stand for $\gamma_\Psi$ and $\alpha_\Psi$ in (40).

Let us first consider the fermionic case. It is straightforward to see that

$$\frac{1}{4} - A_-^2 = \Gamma_\Psi(1-\Gamma_\Psi) = \begin{pmatrix} \gamma(1-\gamma) - \alpha\alpha^* & -\gamma\alpha + \alpha J\gamma J^* \\ -\alpha^*\gamma + J\gamma J^*\alpha^* & J\gamma(1-\gamma)J^* - \alpha^*\alpha \end{pmatrix}$$

is of trace class since both $\gamma$ and $\alpha\alpha^*$ are of trace class operators on $\mathfrak{h}$. Thus $\mathcal{A}_-^2$ admits an eigenbasis for $\mathfrak{h} \oplus \mathfrak{h}^*$. If $u$ is an eigenvector of $\mathcal{A}_-^2$ then $\mathcal{A}_-$ leaves invariant the subspace $\{u, \mathcal{A}u\}$, which is at most 2-dimensional, and hence $\mathcal{A}$ can be diagonalized in this subspace. Thus $\mathcal{A}$ admits an orthonormal eigenbasis for $\mathfrak{h} \oplus \mathfrak{h}^*$ and Lemma 9.6 can be applied to imply that there exixts a fermionic Bogolubov map $\mathcal{V}$ such that $\mathcal{V}^*\mathcal{A}_-\mathcal{V}$, and hence $\mathcal{V}^*\Gamma_\Psi\mathcal{V}$, has eigenvectors $\{u_n \oplus 0\} \cup \{0 \oplus Ju_n\}$.

It remains to show that $\mathcal{V}$ admits a unitary implementation. Assume that under the basis $\{u_n \oplus 0\} \cup \{0 \oplus Ju_n\}$ the diagonal matrix $\mathcal{V}^*\Gamma_\Psi\mathcal{V}$ has the form

$$\mathcal{V}^*\Gamma_\Psi\mathcal{V} = \begin{pmatrix} \lambda_1 & & & & & \\ & \lambda_2 & & & 0 & \\ & & \ddots & & & \\ & & & 1-\lambda_1 & & \\ & 0 & & & 1-\lambda_2 & \\ & & & & & \ddots \end{pmatrix} \tag{74}$$

for $0 \le \lambda_i \le 1/2$ for $i = 1, 2, ....$ Since $\Gamma_\Psi(1-\Gamma_\Psi)$ is of trace class, we must have $\sum_{i=1}^\infty \lambda_i(1-\lambda_i) < \infty$ and hence $\sum_{i=1}^\infty \lambda_i < \infty$. This means that the upper left block of the matrix $\mathcal{V}^*\Gamma_\Psi\mathcal{V}$ has finite trace on $\mathfrak{h}$, i.e.

$$\mathrm{Tr}_\mathfrak{h}[U^*\gamma U + U^*\alpha V + V^*\alpha^*U + V^*V + V^*J\gamma J^*V] < \infty$$

here we use the matrix form (56) for $\mathcal{V}$. It is clear that $U^*\gamma U$ and $V^*J\gamma J^*V$ are of trace class. Using the Cauchy-Schwarz inequality

$$\mathrm{Tr}[XY + Y^*X^*] \le 2(\mathrm{Tr}[X^*X])^{1/2}(\mathrm{Tr}[Y^*Y])^{1/2}$$

we have

$$\begin{aligned} \infty &> \mathrm{Tr}[U^*\alpha V + V^*\alpha^*U + V^*V] \\ &\ge -2(\mathrm{Tr}[U^*U\alpha\alpha^*])^{1/2}(\mathrm{Tr}[V^*V])^{1/2} + \mathrm{Tr}[V^*V]. \end{aligned}$$

Thus $\mathrm{Tr}[V^*V] < \infty$ and Theorem (9.5) ensures that $\mathcal{V}$ admits a unitary implementation $\mathbb{U}_{\mathcal{V}}$.

We turn now on the bosonic case which needs some subtle adjustments. We need to check that $\mathcal{A}_+$ fulfills the conditions of Lemma 9.6. The positivity of $\mathcal{A}_+$ is left as an exericise for the reader. Now we prove that $\mathcal{S}\mathcal{A}_+$ admits an eigenbasis for $\mathfrak{h} \oplus \mathfrak{h}^*$. Because $\mathcal{S}\mathcal{A}_+$ is not a Hermitian we associate it with the Hermitian $C = \mathcal{A}_+^{1/2}\mathcal{S}\mathcal{A}_+^{1/2}$ where $\mathcal{A}_+^{1/2}$ is the square root of the possitive definite operator $\mathcal{A}_+$. Note that $\mathcal{A}_+$ has an orthonormal eigenbasis since $\mathcal{A}_+ - \frac{1}{2}$ is a Hilbert-Schmidt operator, and hence $\mathcal{A}_+^{1/2}$ is well-defined. The point is that if $v$ is an eigenvector of $C$ then $\mathcal{S}\mathcal{A}_+^{1/2}$ is an eigenvector of $\mathcal{S}\mathcal{A}_+$ since $\mathcal{S}\mathcal{A}_+^{1/2}$ is injective and

$$\mathcal{S}\mathcal{A}_+(\mathcal{S}\mathcal{A}_+^{1/2}) = \mathcal{S}\mathcal{A}_+^{1/2}(\mathcal{A}_+^{1/2}\mathcal{S}\mathcal{A}_+^{1/2}) = \mathcal{S}\mathcal{A}_+^{1/2}C.$$

On the other hand, since

$$\begin{aligned} C^2 - \frac{1}{4} &= \mathcal{A}_+^{1/2}(\mathcal{S}\mathcal{A}_+\mathcal{S})\mathcal{A}_+ - \frac{1}{4} \\ &= \mathcal{A}_+^{1/2}\begin{pmatrix} \gamma & -\alpha \\ -\alpha^* & J\gamma J^* \end{pmatrix}\mathcal{A}_+^{1/2} + \frac{1}{2}\begin{pmatrix} \gamma & \alpha \\ \alpha^* & J\gamma J^* \end{pmatrix} \end{aligned}$$

is a Hilbert-Schimidt operator we may argue similarly to the fermionic case to veryfy that $C$ has an orthonormal eigenbasis .

Thus employing Lemma 9.6 we deduce that there exists a bosonic Bogolubov transformation $\mathcal{V}$ such that $\mathcal{V}^*\mathcal{A}_+\mathcal{V}$, and hence $\mathcal{V}^*\Gamma_\Psi\mathcal{V}$, has eigenvectors $\{u_n \oplus 0\} \cup \{0 \oplus Ju_n\}$. We may use the fact that $\Gamma_\Psi\mathcal{S}(\Gamma_\Psi + \mathcal{S})$ has finite trace to prove that the upper left of the matrix $\mathcal{V}^*\Gamma_\Psi\mathcal{V}$ is of trace class on $\mathfrak{h}$ and then process similarly as in the fermionic case to verify that $\mathcal{V}$ admits a unitary implementation. $\square$

Theorem 9.9 may also be rewritten that if $\Gamma_\Psi$ is the 1-pdm of a normalized vector $\Psi \in \mathcal{F}^{B,F}(\mathfrak{h})$ then there exists a Bogolubov map $\mathcal{V}$, which admits a unitary implementation, such that

$$\mathcal{V}^*\Gamma\mathcal{V} = \begin{pmatrix} \xi & 0 \\ 0 & 1 \pm J\xi J^* \end{pmatrix}$$

where $\xi$ is a positive semi-definite trace class operator on $\mathfrak{h}$. In the fermionic case we can impose moreover that $\xi \leq \frac{1}{2}I$.

Correction since August 30, 09: Problem added

**PROBLEM 9.10.** *Show that if* $\Gamma_\Psi$ *is the 1-pdm of a normalized vector* $\Psi$ *in the bosonic Fock space then* $\Gamma_\Psi + \frac{1}{2}\mathcal{S}$ *is positive definite.*

*(Hint: If* $\mathrm{Ker}(\Gamma_\Psi + \frac{1}{2}\mathcal{S})$ *is nontrivial then it includes an element* $f \oplus Jf$ *for some* $f \in \mathfrak{h}\backslash\{0\}$*. It is impossible since* $\Gamma_\Psi \geq 0$*.)*

# 10 Quasi-free pure states

Correction since August 30, 09: Quasi-free states → quasi-free pure states

**DEFINITION 10.1** (Quasi-free pure states)**.** A vector $\Psi \in \mathcal{F}^{\mathrm{F,B}}(\mathfrak{h})$ is called a *quasi-free pure* state if there exists a Bogolubov map $\mathcal{V} : \mathfrak{h}\oplus\mathfrak{h}^* \to \mathfrak{h}\oplus\mathfrak{h}^*$ which is unitarily implementable on $\mathcal{F}^{\mathrm{F,B}}(\mathfrak{h})$ such that $\Psi = \mathbb{U}_{\mathcal{V}}|0\rangle$, where $\mathbb{U}_{\mathcal{V}} : \mathcal{F}^{\mathrm{F,B}}(\mathfrak{h}) \to \mathcal{F}^{\mathrm{F,B}}(\mathfrak{h})$ is the unitary implementation of $\mathcal{V}$.

**THEOREM 10.2** (Wick's Theorem)**.**
*If* $\Psi \in \mathcal{F}^{\mathrm{F,B}}(\mathfrak{h})$ *is a quasi-free pure state and* $F_1, \ldots, F_{2m} \in \mathfrak{h}\oplus\mathfrak{h}^*$ *for* $m \geq 1$ *then*

Correction since June 24: $\pi \to \sigma$

$$\begin{aligned}(\Psi, A_\pm(F_1)\cdots A_\pm(F_{2m})\Psi) = \qquad\qquad\qquad\qquad\qquad\qquad\qquad (75)\\ \sum_{\sigma\in P_{2m}} (\pm 1)^\sigma (\Psi, A_\pm(F_{\sigma(1)})A_\pm(F_{\sigma(2)})\Psi)\cdots(\Psi, A_\pm(F_{\sigma(2m-1)})A_\pm(F_{\sigma(2m)})\Psi),\end{aligned}$$

*and*

$$(\Psi, A_\pm(F_1)\cdots A_\pm(F_{2m-1})\Psi) = 0. \qquad (76)$$

*Here* $P_{2m}$ *is the set of pairings*

$$\begin{aligned}P_{2m} = \{\sigma \in S_{2m} \mid \sigma(2j-1) < \sigma(2j+1), j = 1, \ldots, m-1,\\ \sigma(2j-1) < \sigma(2j),\ j = 1, \ldots, m\}.\end{aligned}$$

Note that the number of pairings is $\frac{(2m)!}{2^m m!}$.

**PROBLEM 10.3.** *Prove Theorem 10.2.*

According to Theorem 10.2 we can calculate all expectations of quasi-free pure states from knowing only the generalized 1-particle density matrix. Recall, in fact, that

Correction since August 30, 09: $\mathcal{V} \to \mathcal{V}^{-1}$.

$$(F_1, \Gamma_\Psi F_2) = (\Psi, A_\pm^*(F_2)A_\pm(F_1)\Psi) = \langle 0|A_\pm^*(\mathcal{V}^{-1}F_2)A_\pm(\mathcal{V}^{-1}F_1)|0\rangle.$$

In particular, we have that the expected particle number of a quasi-free pure state is

Correction since August 30, 09: $U \to U^*, V \to \mp V^*J$ since $\mathbb{U}_{\mathcal{V}}^* A_\pm(F)\mathbb{U}_{\mathcal{V}} = A_\pm(\mathcal{V}^{-1}F)$

$$\begin{aligned}(\Psi, \mathcal{N}\Psi) &= \sum_{i=1}(\Psi, a_\pm^*(f_i)a_\pm(f_i)\Psi)\\ &= \sum_{i=1}\langle 0|(a_\pm^*(U^*f_i) + a_\pm(\mp V^*Jf_i))(a_\pm(U^*f_i) + a_\pm^*(\mp V^*Jf_i))|0\rangle\\ &= \sum_{i=1}\langle 0|(a_\pm(V^*Jf_i)a_\pm^*(V^*Jf_i)|0\rangle = \sum_{i=1}(Vf_i, Vf_i) = \mathrm{Tr}V^*V,\end{aligned}$$

where $(f_i)$ is an orthonormal basis for $\mathfrak{h}$.

We see that the expected particle number is finite since we assume that $V$ satisfies the Shale-Stinespring condition.

In the next theorem we characterize the generalized 1-particle density matrices of quasi-free pure states.

**THEOREM 10.4** (Generalized 1-pdm of quasi-free pure state). *If $\Psi \in \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$ is a quasi-free pure state then the generalized 1-particle density matrix $\Gamma = \Gamma_\Psi : \mathfrak{h}\oplus\mathfrak{h}^* \to \mathfrak{h}\oplus\mathfrak{h}^*$ satisfies*

$$\begin{aligned}&\textit{For fermions: } \Gamma \textit{ is a projection, i.e., } \Gamma^2 = \Gamma\\ &\textit{For bosons: } \Gamma\mathcal{S}\Gamma = -\Gamma.\end{aligned} \tag{77}$$

*Conversely, if $\Gamma : \mathfrak{h}\oplus\mathfrak{h}^* \to \mathfrak{h}\oplus\mathfrak{h}^*$ is a positive semi-definite operator satisfying (77) of the form*

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \pm J\alpha J & 1 \pm J\gamma J^* \end{pmatrix}. \tag{78}$$

*with $\gamma$ a trace class operator, then there is a quasi-free pure state $\Psi \in \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$ such that $\Gamma_\Psi = \Gamma$.*

*Proof.* Since $\Psi$ is a quasi-free pure state we may assume that $\Psi = \mathbb{U}_{\mathcal{V}}|0\rangle$ for a Bogolubov map $\mathcal{V} : \mathfrak{h}\oplus\mathfrak{h}^* \to \mathfrak{h}\oplus\mathfrak{h}^*$. Thus for all $F_1, F_2 \in \mathfrak{h}\oplus\mathfrak{h}^*$ we have according to Theorem 9.5

$$(F_1, \mathcal{V}^*\Gamma_\Psi\mathcal{V}F_2) = (\mathcal{V}F_1, \Gamma_\Psi\mathcal{V}F_2) = (\Psi, A_\pm^*(\mathcal{V}F_2)A_\pm(\mathcal{V}F_1)\Psi) = \langle 0|A_\pm^*(F_2)A_\pm(F_1)|0\rangle.$$

If we write $F_i = f_i \oplus Jg_i$, $i = 1, 2$ we have

$$\langle 0|A_\pm^*(F_2)A_\pm(F_1)|0\rangle = \langle 0|(a_\pm^*(f_2) + a_\pm(g_2))(a_\pm(f_1) + a_\pm^*(g_1)|0\rangle = (g_2, g_1)_{\mathfrak{h}}.$$

We conclude that

$$\mathcal{V}^*\Gamma_\Psi\mathcal{V} = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}.$$

From (54) or (55) we find that

$$\Gamma_\Psi = \mathcal{S}_\pm\mathcal{V}\mathcal{S}_\pm \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} \mathcal{S}_\pm\mathcal{V}^*\mathcal{S}_\pm = \mathcal{S}_\pm\mathcal{V} \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} \mathcal{V}^*\mathcal{S}_\pm,$$

where we have introduced the notation $\mathcal{S}_- = I$ and $\mathcal{S}_+ = \mathcal{S}$. Hence using (54) or (55) we find

$$\Gamma_\Psi\mathcal{S}_\pm\Gamma_\Psi = \mathcal{S}_\pm\mathcal{V} \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} \mathcal{S}_\pm \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} \mathcal{V}^*\mathcal{S}_\pm = \mp\mathcal{S}_\pm\mathcal{V} \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} \mathcal{V}^*\mathcal{S}_\pm = \mp\Gamma_\Psi.$$

To prove the converse assume now that $\Gamma$ is a positive semi-definite Hermitian operator satisfying (77) and of the form (78). Then because $\Gamma \geq 0$ we must have $\alpha = \pm J\alpha J$. Thus applying Theorem 9.9 we may find a (+) bosonic or (-) femionic Bogolubov map $\mathcal{V}$, which admits a unitary implementation $\mathbb{U}_\mathcal{V}$, such that

Correction since August 30, 09: This part of the proof formulated.

$$\mathcal{V}^*\Gamma\mathcal{V} = \begin{pmatrix} \xi & 0 \\ 0 & 1 \pm J\xi J^* \end{pmatrix}$$

where $\xi$ is a positive semi-definite trace class operator on $\mathfrak{h}$ and $\xi \leq \frac{1}{2}I$ in the fermionic case. (Infact, Theorem 9.9 is stated for 1-pdm $\Gamma_\Psi$ of normalized vector $\Psi$ but in the proof we just need the specific form of $\Gamma_\Psi$.) It follows from condition (77) that $\xi(1 \pm \xi) = 0$ and hence $\xi = 0$. Thus $\mathcal{V}^*\Gamma\mathcal{V}$ is just the 1-pdm of the vacuum. Finally it is straightforward to see that $\Gamma$ is the 1-pdm of the quasi-free pure state $\mathbb{U}_\mathcal{V}|0\rangle$. □

# 11 Quadratic Hamiltonians

Correction since August 30, 09: Definition reformulated for infinite dimension

**DEFINITION 11.1** (Quadratic Hamiltonians)**.** Let $\mathcal{A} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ be a Hermitian, trace class operator and assume moreover in the bosonic case that it is positive semi-definite. The operator

$$H_\mathcal{A}^\pm = \sum_{i,j=1}^{2M} (F_i, \mathcal{A}F_j)A_\pm^*(F_i)A_\pm(F_j),$$

where $F_1, \ldots, F_{2M}$ is an orthonormal basis for $\mathfrak{h} \oplus \mathfrak{h}^*$ is called a bosonic (+) of fermionic (−) *quadratic Hamiltonian* corresponding to $\mathcal{A}$.

**PROBLEM 11.2.** *Show that $H^{\pm}_{\mathcal{A}}$ is Hermitian and is independent of the choice of basis for $\mathfrak{h} \oplus \mathfrak{h}^*$ used to define it.*

**PROBLEM 11.3.** *Show that $H^{+}_{\mathcal{A}} \geq 0$ and $H^{-}_{\mathcal{A}} \geq \mathrm{Tr}[\mathcal{A}_-]$, where $\mathrm{Tr}[\mathcal{A}_-]$ is the sum of all negative eigenvalue of $\mathcal{A}$. (Hint: $(\Psi, H^{\pm}_{\mathcal{A}}\Psi) = \mathrm{Tr}[\mathcal{A}\Gamma_\Psi]$.)*

Correction since August 30, 09: Problem added

Thus the quadratic Hamiltonian $H^{\pm}_{\mathcal{A}}$ is bounded from below and we may consider its ground state energy. The point is that to determine the ground state energy for a quadratic Hamiltonians it suffices to consider the quasi-free pure states.

**LEMMA 11.4.** *If $\mathcal{A} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ is Hermitian, trace class (and positive semi-definite in the bosonic case) we may find a Hermitian, trace class operator $\mathcal{A}' : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ (which is positive definite in the bosonic case) satisfying $\mathcal{J}\mathcal{A}'\mathcal{J} = \pm\mathcal{A}'$ (+ in the bosonic case and − in the fermionic case) such that*

Correction since June 24: sign corrected in (79)

$$H^{\pm}_{\mathcal{A}'} = H^{\pm}_{\mathcal{A}} \pm \tfrac{1}{2}\mathrm{Tr}(\mathcal{A}\mathcal{S}_\pm)I, \tag{79}$$

*where $\mathcal{S}_+ = \mathcal{S}$ and $\mathcal{S}_- = I$.*

*Proof.* Using the CCR or CAR relations (47) and (48) we have

$$\begin{aligned} H^{\pm}_{\mathcal{A}} &= \pm \sum_{i,j=1}^{2M} (F_i, \mathcal{A}F_j) A_\pm(F_j) A^*_\pm(F_i) \mp \sum_{i,j=1}^{2M} (F_i, \mathcal{A}F_j)(F_j, \mathcal{S}_\pm F_i) \\ &= \pm \sum_{i,j=1}^{2M} (F_i, \mathcal{A}F_j) A^*_\pm(\mathcal{J}F_j) A_\pm(\mathcal{J}F_i) \mp \mathrm{Tr}(\mathcal{A}\mathcal{S}_\pm) \end{aligned}$$

where we have also applied (46).

If we now use that from (89)

$$(F_i, \mathcal{A}F_j) = (\mathcal{A}F_i, F_j) = (\mathcal{J}\mathcal{J}\mathcal{A}\mathcal{J}\mathcal{J}F_i, F_j) = (\mathcal{J}F_j, \mathcal{J}\mathcal{A}\mathcal{J}\mathcal{J}F_i)$$

we get

$$H^{\pm}_{\mathcal{A}} = \pm \sum_{i,j=1}^{2M} (\mathcal{J}F_j, \mathcal{J}\mathcal{A}\mathcal{J}\mathcal{J}F_i) A^*_\pm(\mathcal{J}F_j) A_\pm(\mathcal{J}F_i) - \mathrm{Tr}(\mathcal{A}\mathcal{S}_\pm) = \pm H^{\pm}_{\mathcal{J}\mathcal{A}\mathcal{J}} \mp \mathrm{Tr}(\mathcal{A}\mathcal{S}_\pm).$$

The last equality follows since $\mathcal{J}F_1, \ldots, \mathcal{J}F_{2M}$ is an orthonormal basis for $\mathfrak{h}\oplus\mathfrak{h}^*$. Thus if we define $\mathcal{A}' = \frac{1}{2}(\mathcal{A}\pm\mathcal{J}\mathcal{A}\mathcal{J})$ we have $\mathcal{J}\mathcal{A}'\mathcal{J} = \pm\mathcal{A}'$ and the relation (79) holds. □

**THEOREM 11.5** (Variational principle for quadratic Hamiltonian)**.**
*If $\mathcal{A} : \mathfrak{h}\oplus\mathfrak{h}^* \to \mathfrak{h}\oplus\mathfrak{h}^*$ is Hermitian, trace class (and positive semi-definite in the bosonic case) and*

Correction since June 24: Theorem added

$$E^{H^{\pm}_{A}} := \inf\{(\Psi, H^{\pm}_{\mathcal{A}}\Psi) | \Psi \in \mathcal{F}^{B,F}(\mathfrak{h}), \|\Psi\| = 1\}$$

*denotes the true ground state energy of the quadratic Hamiltonian $H^{\pm}_{A}$ then*

$$E^{H^{\pm}_{A}} = \inf\{(\Psi, H^{\pm}_{\mathcal{A}}\Psi) | \Psi \in \mathcal{F}^{B,F}(\mathfrak{h}) \text{ is a quasi} - \text{free pure state}\}.$$

*Proof.* By a simple approximation we can consider the ground state energy $E^{H^{\pm}_{A}}$ as the infimum over normalized vector $\Psi \in \mathcal{F}^{B,F}(\mathfrak{h})$ with finite particle expectation. The result thus follows if we prove in this case that there exists a quasi-free pure state $\widetilde{\Psi}$ such that

$$(\widetilde{\Psi}, H^{\pm}_{\mathcal{A}}\widetilde{\Psi}) \leq (\Psi, H^{\pm}_{\mathcal{A}}\Psi).$$

Due to Lemma 11.4 we may assume that $\mathcal{J}\mathcal{A}\mathcal{J} = \pm\mathcal{A}$ (and $\mathcal{A} \geq 0$ in the bosonic case). Moreover using Theorem 9.9 we may represent $\Gamma_\Psi$, the 1-pdm of $\Psi$, by

$$\Gamma_\Psi = \mathcal{V}_\Psi \begin{pmatrix} \xi & 0 \\ 0 & 1 \pm J\xi J^* \end{pmatrix} \mathcal{V}^*_\Psi$$

where $\mathcal{V}_\Psi$ is a Bogolubov map, which admits a unitary implementation, and $\xi : \mathfrak{h} \to \mathfrak{h}$ is a positive semi-definite trace class operator.

Thus

$$\begin{aligned} (\Psi, H^{\pm}_{\mathcal{A}}\Psi) = \mathrm{Tr}[\mathcal{A}\Gamma_\Psi] &= \mathrm{Tr}\left[\mathcal{A}\mathcal{V}_\Psi \begin{pmatrix} \xi & 0 \\ 0 & 1 \pm J\xi J^* \end{pmatrix} \mathcal{V}^*_\Psi\right] \\ &= \mathrm{Tr}\left[\mathcal{V}^*_\Psi\mathcal{A}\mathcal{V}_\Psi \begin{pmatrix} \xi & 0 \\ 0 & 1 \pm J\xi J^* \end{pmatrix}\right]. \end{aligned}$$

Because $J\mathcal{A}J = \pm\mathcal{A}$ and $JcV_\Psi J = \mathcal{V}_\Psi$, we also have

$$J\mathcal{V}^*_\Psi\mathcal{A}\mathcal{V}_\Psi J = \pm\mathcal{V}^*_\Psi\mathcal{A}\mathcal{V}_\Psi$$

and hence we may write $\mathcal{V}_\Psi^*\mathcal{A}\mathcal{V}_\Psi$ in the block form

$$\mathcal{V}_\Psi^*\mathcal{A}\mathcal{V}_\Psi = \begin{pmatrix} a & J^*bJ^* \\ b & \pm JaJ^* \end{pmatrix}$$

where $a$ is a Hermitian, trace class operator on $\mathfrak{h}$. Thus

$$(\Psi, H_\mathcal{A}^\pm\Psi) = \mathrm{Tr}\left[\begin{pmatrix} a & J^*bJ^* \\ b & \pm JaJ^* \end{pmatrix}\begin{pmatrix} \xi & 0 \\ 0 & 1\pm J\xi J^* \end{pmatrix}\right] = 2\mathrm{Tr}_\mathfrak{h}[a\xi] \pm \mathrm{Tr}[a].$$

We first consider the bosonic case. Since $\mathcal{A} \geq 0$ we must have $a \geq 0$ and hence $\mathrm{Tr}[a\xi] \geq 0$ since $\xi \geq 0$. On the other hand, due to Theorem 10.4 there exists a quasi-free pure state $\widetilde{\Psi}$ whose 1-pdm is

$$\mathcal{V}_\Psi \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} V_\Psi^*.$$

Thus we get

$$(\Psi, H_\mathcal{A}^\pm\Psi) - (\widetilde{\Psi}, H_\mathcal{A}^\pm\widetilde{\Psi}) = 2\mathrm{Tr}[a\xi] \geq 0.$$

For the fermionic case we have $0 \leq \xi \leq 1$. Thus we can choose $\xi' = \chi_{(-\infty,0)}(a)$, i.e. $\xi' = \sum_{\lambda_i<0} \langle u_i|$ for an orthogonal eigenbasis $u_i$ of $a$ corresponding to eigenvalues $\lambda_i$. Because $\xi' = (\xi')^2$ we may apply Theorem 10.4 to find a quasi-free pure state $\widetilde{\Psi}$ whose 1-pdm is

$$\mathcal{V}_\Psi \begin{pmatrix} \xi' & 0 \\ 0 & 1+J\xi' J^* \end{pmatrix} \mathcal{V}_\Psi^*.$$

It is straightforward to see that

$$(\Psi, H_\mathcal{A}^\pm\Psi)\ (\widetilde{\Psi}, H_\mathcal{A}^\pm\widetilde{\Psi}) = 2\mathrm{Tr}[a(\xi-\xi')] \geq 0$$

since $a(\xi-\xi') = a(1-\xi')\xi - a\xi'(1-\xi) \geq 0$. Here we used $a(1-\xi') \geq 0$ and $a\xi' \leq 0$. □

Note that the above theorem says nothing about the existence of a ground state for the quadratic Hamiltonian. In the next theorem for simplicity we assume that $\mathfrak{h}$ is finite dimensional.

**THEOREM 11.6** (Ground state eigenvector for quadratic Hamiltonian)**.** *Assume that $\mathfrak{h}$ is finite dimensional. Let $\mathcal{A} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ be a Hermitian operator and assume moreover in the bosonic case that it is positive definite. Then the quadratic Hamiltonian has a ground state eigenvector which is a quasi-free pure state. Moreover in the bosonic case the ground state is unique in the class of quasi-free pure state.*

*REMARK* 11.7. If $\mathcal{A}$ is only positive *semi*-definite then the quadratic bosonic Hamiltonian $H^+_{\mathcal{A}}$ Hamiltonian may not have a ground state eigenvector.

*Proof.* Due to Lemma 11.4 we may assume that $\mathcal{J}\mathcal{A}\mathcal{J} = \pm\mathcal{A}$ (and $\mathcal{A}$ is positive definite in the bosonic case). Thus employing Lemma 9.6 we may represent, under an orthogonal basis $\{u_n \oplus 0\} \cup \{0 \oplus Ju_n\}$,

$$\mathcal{A} = \mathcal{V}^*_{\mathcal{A}} \begin{pmatrix} d & 0 \\ 0 & \pm JdJ^* \end{pmatrix} \mathcal{V}_{\mathcal{A}}$$

where $\mathcal{V}_{\mathcal{A}}$ is a (+) bosonic or (-) fermionic Bogolubov map and $d : \mathfrak{h} \to \mathfrak{h}$ is positive semi-definite (positive definite in the bosonic case). Moreover, because $\mathfrak{h}$ is finite dimensional the Shale-Stinespring condition holds and hence $\mathcal{V}$ admits a unitary implementation.

Thus for any normalized vector $\Psi \in \mathcal{F}^{B,F}(\mathfrak{h})$ we have

$$(\Psi, H^{\pm}_{\mathcal{A}}\Psi) = \mathrm{Tr}[\mathcal{A}\Gamma_\Psi] = \mathrm{Tr}\left[\mathcal{V}^*_{\mathcal{A}} \begin{pmatrix} d & 0 \\ 0 & \pm d \end{pmatrix} \mathcal{V}_{\mathcal{A}}\Gamma_\Psi\right] = \mathrm{Tr}\left[\begin{pmatrix} d & 0 \\ 0 & \pm d \end{pmatrix} \mathcal{V}_{\mathcal{A}}\Gamma_\Psi\mathcal{V}^*_{\mathcal{A}}\right].$$

We may write $\mathcal{V}_{\mathcal{A}}\Gamma_\Psi\mathcal{V}^*_{\mathcal{A}}$ in the block form

$$\mathcal{V}_{\mathcal{A}}\Gamma_\Psi\mathcal{V}^*_{\mathcal{A}} = \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 \pm J\gamma J^* \end{pmatrix}$$

where $\gamma : \mathfrak{h} \to \mathfrak{h}$ is positive semi-definite. Thus

$$\begin{aligned} (\Psi, H^{\pm}_{\mathcal{A}}\Psi) &= \mathrm{Tr}\left[\begin{pmatrix} d & 0 \\ 0 & \pm d \end{pmatrix}\begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 \pm J\gamma J^* \end{pmatrix}\right] \\ &= 2\mathrm{Tr}_{\mathfrak{h}}[d\gamma] \pm \mathrm{Tr}_{\mathfrak{h}}[d] \geq \pm\mathrm{Tr}_{\mathfrak{h}}[d]. \end{aligned}$$

The equality occurs if $\gamma = 0$ (this is unique for bosons but may not be unique for fermions). The conclusion that $\mathbb{U}^*_{\mathcal{V}_{\mathcal{A}}}|0\rangle$ is a ground state for the Hamiltonian $H^{\pm}_{\mathcal{A}}$ is left as an exercise for the readers. □

**PROBLEM 11.8** (Quadratic Hamiltonians and Bogolubov unitaries). *If $\mathcal{V} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ is a Bogolubov map and $\mathbb{U}_{\mathcal{V}} : \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h}) \to \mathcal{F}^{\mathrm{B,F}}(\mathfrak{h})$ is the corresponding unitary implementation then for all Hermitian $\mathcal{A} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ we have*

Correction since August 30, 09: Theorem → Exercise

Correction since June 24: $\mathcal{V}$ and $\mathcal{V}^*$ interchanged

$$\mathbb{U}_{\mathcal{V}} H^{\pm}_{\mathcal{A}} \mathbb{U}^*_{\mathcal{V}} = H^{\pm}_{\mathcal{V}\mathcal{A}\mathcal{V}^*}.$$

**PROBLEM 11.9.** *Let $\mathfrak{h} = \mathbb{C}^2$ and let $a_{1\pm} = a_{\pm}(1,0)$ and $a_{2\pm} = a_{\pm}(0,1)$. Find the ground state energy and ground state of the two Hamiltonians*

Correction by July 6 Hamiltonian corrected

$$H_{\pm} = (1+b)(a^*_{1\pm}a_{1\pm} + a^*_{2\pm}a_{2\pm}) + b(a^*_{1\pm}a^*_{2\pm} + a_{2\pm}a_{1\pm})$$

*where $b > 0$.*

# 12 Generalized Hartree-Fock Theory

Generalized Hartree-Fock theory is a theory for studying interacting fermions. In generalized Hartree-Fock theory one restricts attention to quasi-free pure states. According to Theorem 10.4 the set of all 1-particle density matrices of quasi-free fermionic pure states is[15]

Corrections since June 24: $\mathcal{G}^{\mathrm{HF}}$ redefined

$$\mathcal{G}^{\mathrm{HF}} = \left\{\Gamma : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^* \mid \Gamma^* = \Gamma \text{ has the form (43)}\ ,\ \Gamma^2 = \Gamma,\ \mathrm{Tr}\gamma < \infty\right\}.$$

Let us for $\Gamma \in \mathcal{G}^{\mathrm{HF}}$ denote by $\Psi_\Gamma \in \mathcal{F}^{\mathrm{F}}(\mathfrak{h})$ the (normalized) quasi-free fermionic state having $\Gamma$ as its 1-particle density matrix.

We consider a fermionic operator in the grand canonical picture, i.e., an operator on the Fock space $\mathcal{F}^{\mathrm{F}}(\mathfrak{h})$

$$H = \bigoplus_{N=0}^{\infty} \left( \sum_{i=1}^{N} h_i + \sum_{1 \le i < j \le N} W_{i,j} \right). \tag{80}$$

**DEFINITION 12.1** (Generalized Hartree-Fock theory). The generalized Hartree-Fock functional for the operator $H$ is map $\mathcal{E}^{\mathrm{HF}} : \mathcal{G}^{\mathrm{HF}} \to \mathbb{R}$ defined by

$$\mathcal{E}^{\mathrm{HF}}(\Gamma) = (\Psi_\Gamma, H\Psi_\Gamma).$$

[15] We need no longer assume that $\mathfrak{h}$ is finite dimensional

The Hartree-Fock ground state energy is

$$E^{\mathrm{HF}} = \inf\{\mathcal{E}^{\mathrm{HF}}(\Gamma) \mid \Gamma \in \mathcal{G}^{\mathrm{HF}}\}.$$

If $E^{\mathrm{HF}} = \mathcal{E}^{\mathrm{HF}}(\Gamma_0)$ we call $\Gamma_0$ (and $\Psi_{\Gamma_0}$) for a Hartree-Fock ground state.

There are several results in the mathematical physics literature that establish existence of a minimizer of the generalized Hartree-Fock functional. There are also several results on how well the Hartree-Fock energy approximates the true ground state energy. Since the generalized Hartree-Fock energy is found by minimizing over a restricted set of states we have the following obvious result.

**THEOREM 12.2** (Hartree-Fock energy upper bound on true energy)**.** *If*

$$E^{\mathrm{F}} = \inf\{(\Psi, H\Psi) \mid \Psi \in \mathcal{F}^{\mathrm{F}}(\mathfrak{h}), \|\Psi\| = 1\}$$

*denotes the true fermionic ground state energy and $E^{\mathrm{HF}}$ the Hartree-Fock ground state energy for the Hamiltonian $H$ we have*

$$E^{\mathrm{F}} \leq E^{\mathrm{HF}}.$$

Hartree-Fock theory has been widely used in chemistry to calculate the energy and structure of atoms and molecules. It is fairly successful but has over the years been generalized in various ways.

Using Theorem 10.2 we may calculate $\mathcal{E}^{\mathrm{HF}}(\Gamma)$ explicitly. Assume that $\Gamma$ is written in the form (43), i.e.,

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 - J\gamma J^* \end{pmatrix}, \tag{81}$$

It is convenient to introduce the vector $\widetilde{\alpha} \in \mathfrak{h} \otimes \mathfrak{h}$ by

Correction since June 24: $\oplus \to \otimes$ several places

$$(f \otimes g, \widetilde{\alpha})_{\mathfrak{h}\otimes\mathfrak{h}} = (f, \alpha_{\Psi_\Gamma} Jg) = (\Psi_\Gamma, a_-(g)a_-(f)\Psi_\Gamma).$$

A straightforward calculation using Theorem 10.2 then shows that

Correction since June 24: Parentheses included

$$\mathcal{E}^{\mathrm{HF}}(\Gamma) = \mathrm{Tr}_{\mathfrak{h}}[h\gamma] + \tfrac{1}{2}\mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}[W(\gamma\otimes\gamma - \mathrm{Ex}\gamma\otimes\gamma)] + \tfrac{1}{2}(\widetilde{\alpha}, W\widetilde{\alpha})_{\mathfrak{h}\otimes\mathfrak{h}}. \tag{82}$$

**PROBLEM 12.3.** *Prove (82) using that if we choose an orthonormal basis $u_1, u_2, \ldots$ for $\mathfrak{h}$ and denote $a_-(u_i) = a_i$ we may write the operator $H$ in second quantized form according to (25) and (27) as*

$$H = \sum_{i,j=1} (u_i, hu_j) a_i^* a_j + \tfrac{1}{2} \sum_{i,j,\mu,\nu} (u_i \otimes u_j, W u_\mu \otimes u_\nu) a_i^* a_j^* a_\nu a_\mu.$$

If $\alpha = 0$ we say that $\Gamma$ represents a normal Hartree-Fock state. In this case $\Psi_\Gamma$ is a Slater determinant. If $\alpha \neq 0$ we call the state $\Psi_\Gamma$ a BCS state after Bardeen, Cooper and Schrieffer (see footnote 13 on Page 46) who used these type of states to explain the phenomenon of super-conductivity.

We now mention without proof a result that implies that if $W \geq 0$ we may restrict to normal states.

**THEOREM 12.4.** *If $W \geq 0$ then*

$$E^{\mathrm{HF}} = \inf\{\mathcal{E}^{\mathrm{HF}}(\Gamma) \mid \Gamma \in \mathcal{G}^{\mathrm{HF}}, \Gamma \text{ has the form (81) with } \alpha = 0\}.$$

It is important in the BCS theory of superconductivity that the minimizing Hartree-Fock state is not normal. For this reason it is important to understand where an attractive (negative) two-body interaction between electrons may come from. It turns out that such an attraction may be explained because of the interaction of the electrons with the atoms in the superconducting material. More precisely, it has to do with the vibrational modes that the electrons excite in the crystal of atoms.

# 13 Bogolubov Theory

Bogolubov theory is the bosonic analogue of Hartree-Fock theory. We consider again a Hamiltonian of the form (80) but now on the bosonic Fock space $\mathcal{F}^{\mathrm{B}}(\mathfrak{h})$.

In Bogolubov theory one however does not restrict to quasi-free pure states, but to a somewhat extended class. To explain this we need a result whose proof we leave as an exercise to the reader.

**THEOREM 13.1.** *If $\phi \in \mathfrak{h}$ there exists a unitary $\mathbb{U}_\phi : \mathcal{F}^{\mathrm{B}}(\mathfrak{h}) \to \mathcal{F}^{\mathrm{B}}(\mathfrak{h})$ such that for all $f \in \mathfrak{h}$*

$$\mathbb{U}_\phi^* a_+(f) \mathbb{U}_\phi = a_+(f) + (f, \phi).$$

**PROBLEM 13.2.** *Prove Theorem 13.1. Hint: You may proceed as in the proof of Theorem 9.5 (or one may proceed from an entirely algebraic point of view).*

In Bogolubov theory we restrict to states of the form $\mathbb{U}_\phi \mathbb{U}_\mathcal{V}|0\rangle$, where $\phi \in \mathfrak{h}$ and $\mathcal{V} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ is a Bogolubov map. Another way to say this is to first perform a unitary transformation $\mathbb{U}_\phi^* H \mathbb{U}_\phi$ and then to restrict to quasi-free pure states.

*REMARK* 13.3. We saw in Section 11 that quadratic Hamiltonians have quasi-free ground states. If, in the bosonic case, we allow the quadratic operators to have terms that are linear in creation and annihilation operators then the ground states belong to the larger class of vectors for the form $\mathbb{U}_\phi \mathbb{U}_\mathcal{V}|0\rangle$.

According to Theorem 10.4 the set of all 1-particle density matrices of quasi-free bosonic pure states is

Corrections since June 24: Definition of $\mathcal{G}^{\rm Bo}$ changed

$$\mathcal{G}^{\rm Bo} = \{\Gamma : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^* \mid \Gamma \text{ has the form (43)}\ , \Gamma \geq 0,\ \Gamma \mathcal{S} \Gamma = -\Gamma, \mathrm{Tr}\gamma < \infty\}\,.$$

Let us for $\Gamma \in \mathcal{G}^{\rm Bo}$ denote by $\Psi_\Gamma \in \mathcal{F}^{\rm B}(\mathfrak{h})$ the (normalized) quasi-free bosonic state having $\Gamma$ as its 1-particle density matrix.

**DEFINITION 13.4** (Bogolubov theory)**.** The Bogolubov functional for the operator $H$ is the map $\mathcal{E}^{\rm Bo} : \mathcal{G}^{\rm Bo} \times \mathfrak{h} \to \mathbb{R}$ defined by

$$\mathcal{E}^{\rm Bo}(\Gamma, \phi) = (\Psi_\Gamma, \mathbb{U}_\phi^* H \mathbb{U}_\phi \Psi_\Gamma).$$

The Bogolubov ground state energy is

$$E^{\rm Bo} = \inf\{\mathcal{E}^{\rm Bo}(\Gamma, \phi) \mid \Gamma \in \mathcal{G}^{\rm Bo},\ \phi \in \mathfrak{h}\}.$$

If $E^{\rm Bo} = \mathcal{E}^{\rm Bo}(\Gamma_0, \phi_0)$ we call $(\Gamma_0, \phi_0)$ (and $U_{\phi_0}\Psi_{\Gamma_0}$) for a Bogolubov ground state.

As for the Hartree-Fock energy we also have that the Bogolubov energy is an upper bound on the true energy.

**THEOREM 13.5** (Bogolubov energy upper bound on true energy)**.** *If*

$$E^{\rm B} = \inf\{(\Psi, H\Psi) \mid \Psi \in \mathcal{F}^{\rm B}(\mathfrak{h}), \|\Psi\| = 1\}$$

*denotes the true bosonic ground state energy and $E^{\rm Bo}$ the Bogolubov ground state energy for the Hamiltonian $H$ we have*

$$E^{\rm B} \leq E^{\rm Bo}.$$

We leave it to the reader to use Theorem 10.2 to explicitly express the Bogolubov energy in terms of the components $\gamma$ and $\alpha$ of $\Gamma$.

*REMARK* 13.6. In 1967 F. Dyson[16] used Bogolubov theory to prove that a system of charged bosons does not satisfy stability of the second kind. Correction since June 24: Footnote changed

## 13.1 The Bogolubov approximation

We shall finish this section by explicitly discussing an approximation introduced by Bogolubov in his study of superfluidity. We will consider bosons moving on a 3-dimensional torus of size $L > 0$. We identify the torus with $[0, L)^3$.

The Hilbert space is $\mathfrak{h} = L^2([0, L)^3)$. We have an orthonormal basis given by

$$u_p(x) = L^{-3/2}\exp(ipx),\ p \in \frac{2\pi}{L}\mathbb{Z}^3.$$

We have the one-body operator $h = -\Delta - \mu$ where $-\Delta$ is the Laplacian with periodic boundary conditions and $\mu > 0$ is simply a parameter (the *chemical potential*). This means that

$$hu_p = (p^2 - \mu)u_p.$$

For the two-body potential we shall use a function that depends only on the distance between the particles. More precisely on the distance on the torus, i.e, on

$$\min_{k\in\mathbb{Z}^3} |x - y - Lk|.$$

This means we have

$$(u_p \otimes u_q, W u_{p'} \otimes u_{q'}) = L^{-3}\widehat{W}(p - p')\delta_{p+q,p'+q'},$$

where we have introduced the Fourier coefficients of $W$

$$\widehat{W}(k) = \int_{[0,L)^3} W(x)\exp(-ikx)dx.$$

[16] Dyson, Freeman J., Ground state energy of a finite system of charged particles, *Jour. Math. Phys.* **8**, 1538–1545 (1967) Dyson's result has been improved to give the exact asymptotic energy in the large particle limit for a system of charged bosons see E.H. Lieb and J.P. Solovej, Ground State Energy of the Two-Component Charged Bose *Gas. Commun. Math. Phys.* 252, 485 - 534, (2004) and J.P. Solovej, Upper Bounds to the Ground State Energies of the One- and Two-Component Charged Bose Gases. *Commun. Math. Phys.* **266**, No. 3, 797-818, 2006

Let us write $a_+(u_p) = a_p$. We may then express the Hamiltonian in second quantized form as

$$H = \sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3}(p^2-\mu)a_p^*a_p + \frac{1}{2L^3}\sum_{k,p,q\in\frac{2\pi}{L}\mathbb{Z}^3}\widehat{W}(k)a_{p+k}^*a_{q-k}^*a_qa_p.$$

We shall now explain the Bogolubov approximation for this Hamiltonian. Let $\lambda > 0$ be a parameter. We define $H_\lambda = \mathbb{U}_{\lambda u_0}^* H \mathbb{U}_{\lambda u_0}$. Then (where all sums are over $\frac{2\pi}{L}\mathbb{Z}^3$)

$$\begin{aligned} H_\lambda &= \sum_p (p^2-\mu)a_p^*a_p + \frac{1}{2L^3}\sum_{k,p,q}\widehat{W}(k)a_{p+k}^*a_{q-k}^*a_qa_p \\ &\quad -\mu\lambda(a_0+a_0^*) - \lambda^2\mu + \frac{\lambda^4}{2L^3}\widehat{W}(0) + \frac{\lambda^3}{L^3}\widehat{W}(0)(a_0+a_0^*) \\ &\quad +\frac{\lambda^2}{L^3}\widehat{W}(0)\sum_p a_p^*a_p + \frac{\lambda^2}{2L^3}\sum_p \widehat{W}(p)(a_p^*a_p + a_{-p}^*a_{-p} + a_p^*a_{-p}^* + a_pa_{-p}) \\ &\quad +\frac{\lambda}{2L^3}\sum_{p,q}\widehat{W}(p)(2a_{q+p}^*a_qa_p + a_{p+q}^*a_{-p}^*a_q + a_p^*a_{q-p}^*a_q). \end{aligned} \tag{83}$$

The motivation for using the transformation $\mathbb{U}_{\lambda u_0}$ is that one believes that most particles occupy the state $u_0$, called the condensate. After the transformation we look for states to restrict to the subspace where $a_0^*a_0 = 0$. Thus $\lambda^2$ is the expected number of particles in the condensate. We choose $\lambda$ to minimize the two constant terms above, without creation or annihilation operators, i.e., $-\lambda^2\mu + \frac{\lambda^4}{2L^3}\widehat{W}(0)$. Thus we choose $\lambda$ such that $\mu = \frac{\lambda^2}{L^3}\widehat{W}(0)$. Then

Correction since June 24: Choice of $\lambda$ explained

$$\begin{aligned} H_\lambda &= \sum_p p^2 a_p^*a_p + \frac{1}{2L^3}\sum_{k,p,q}\widehat{W}(k)a_{p+k}^*a_{q-k}^*a_qa_p - \frac{\lambda^4}{2L^3}\widehat{W}(0) \\ &\quad +\frac{\lambda^2}{2L^3}\sum_p \widehat{W}(p)(a_p^*a_p + a_{-p}^*a_{-p} + a_p^*a_{-p}^* + a_pa_{-p}) \\ &\quad +\frac{\lambda}{2L^3}\sum_{p,q}\widehat{W}(p)(2a_{q+p}^*a_qa_p + a_{p+q}^*a_{-p}^*a_q + a_p^*a_{q-p}^*a_q). \end{aligned} \tag{84}$$

After the unitary transformation $\mathbb{U}_\lambda$ with the specific choice of $\lambda$ one would guess that the ground state should in some sense be close to the vacuum state. Bogolubov argues therefore that one may think of the operators $a_p$ and $a_p^*$ as being small. For this reason Bogolubov prescribes that one should ignore the terms with 3 and 4 creation and annihilation operators. This approximation, called the Bogolubov approximation, has only been mathematically justified in a few limiting cases for specific interactions. If we nevertheless perform this approximation we arrive at the quadratic Hamiltonian

$$\begin{aligned}\widetilde{H}_\lambda &= \tfrac{1}{2}\sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3}\Big[p^2(a_p^*a_p + a_{-p}^*a_{-p}) \\ &\quad + \frac{\lambda^2}{L^3}\widehat{W}(p)(a_p^*a_p + a_{-p}^*a_{-p} + a_p^*a_{-p}^* + a_pa_{-p})\Big] - \frac{\lambda^4}{2L^3}\widehat{W}(0). \qquad (85)\end{aligned}$$

Since this Hamiltonian is quadratic it has a quasi-free state as ground state. This is one of the motivations why one for the original Hamiltonian restricts attention to these states.

Correction since June 24: Problem reformulated

**PROBLEM 13.7.** *(a) Show that the ground state energy of the quadratic Hamiltonian $2a_0^*a_0 + a_0^*a_0^* + a_0a_0$ is $-1$. (Hint: Use the result of Problem 7.6 to identify $a_0^* + a_0$ with the multiplication operator $\sqrt{2}x$ on the space $L^2(\mathbb{R})$.)*

*(b) Assume that $W(x)$ is smooth with compact support and that $\widehat{W}(p) \geq 0$ and $\widehat{W}(0) > 0$. Use the method described in Section 11, in particular, Problem 11.9, to calculate the ground state energy of $\widetilde{H}_\lambda$.*

*(c) If we keep $\mu$ fixed what is then the ground state energy per volume in the limit as $L \to \infty$? (You may leave your answer as an integral.)*

# A Extra Problems

## A.1 Problems to Section 1

**A.1.1.** Show that (4) defines a bounded operator $K$.

**A.1.2.** (Difficult) Show that $K$ is a compact operator on a Hilbert space if and only if it maps the closed unit ball to a compact set.

Hint to the "if" part:

1. Show that there exists a normalized vector $u_1$ that maximizes $\|Ku_1\|$.
2. Show that $u_1$ is an eigenvector for $K^*K$ (see the hint to Problem 2.5)
3. By induction show that there exists an orthonormal family $u_1, u_2, \ldots$ of eigenvectors of $K^*K$ that span the closure of the range of $K^*K$, which is the orthogonal complement of the kernel of $K^*K$.
4. Show that (4) holds with $\lambda_n = \|Ku_n\|$ and $v_n = \|Ku_n\|^{-1}Ku_n$ (remember to check that $v_1, v_2 \ldots$ is an orthonormal family)

Hint to the "only if" part: Assume $K$ can be written in the form (4). Let $\phi_1, \phi_2, \ldots$ be a sequence of vectors from the closed unit ball. By the Banach-Alouglu Theorem for Hilbert spaces (Corollary B.2 below) there is a weakly convergent subsequence $\phi_{n_1}, \phi_{n_2}, \ldots$ with a weak limit point $\phi$ in the closed unit ball. Show that $\lim_{k\to\infty} K\phi_{n_k} = K\phi$ strongly. Conclude that the image of the closed unit ball by the map $K$ is compact.

**A.1.3.** Use the result of the previous problem to show that the sum of two compact operators is compact. (This is unfortunately not immediate from Definition 1.16.)

**A.1.4.** Assume that $0 \leq \mu_n \leq 1$ for $n = 1, 2, \ldots$ with $\sum_{n=1}^{\infty} \mu_n = 1$ and $\phi_n$, $n = 1, 2, \ldots$ are unit vectors in a Hilbert space $\mathcal{H}$.

(a) Show that the map $\Gamma : \mathcal{H} \to \mathcal{H}$ given by

$$\Gamma u = \sum_{n=1}^{\infty} \mu_n (\phi_n, u)\phi_n$$

is compact and symmetric. [Hint: Use the characterization in Problem A.1.2 (repeat the argument in the “only if” part)].

(b) Show that $\Gamma$ is trace class with $\mathrm{Tr}\Gamma = 1$.

**A.1.5.** Let $\sigma \in S_N$ and $U_\sigma : \bigotimes^N \mathcal{H} \to \bigotimes^N \mathcal{H}$ be the unitary defined in Subsection 1.1. Show that

$$U_\sigma U_\tau = U_{\tau\sigma}.$$

**A.1.6.** For $N \geq 2$ show that

$$\bigotimes_{\mathrm{Sym}}^{N} \mathcal{H} \perp \bigwedge^{N} \mathcal{H}.$$

**A.1.7.** With the notation of Subsection 1.1 show that for all $\sigma \in S_N$

$$U_\sigma P_\pm = (\pm 1)^\sigma P_\pm.$$

What does this mean for the action of $U_\sigma$ on $\bigotimes_{\mathrm{Sym}}^N \mathcal{H}$ and on $\bigwedge^N \mathcal{H}$?

**A.1.8.** Show that if $K$ maps bounded sequences converging weakly to zero in sequences converging strongly to 0 then $K$ is compact. [Hint use the characterization in Problem A.1.2.]

Correction since May 3 Two problems added.

**A.1.9.** Show that if $K$ is an operator on a Hilbert space such that

$$\sum_{k=1}^{\infty} \|K\phi_k\|^2 < \infty$$

for some orthonormal basis $\{\phi_k\}_{k=1}^\infty$ then $K$ is Hilbert Schmidt. [Hint: use the result of the previous problem to show that $K^*$ is compact and hence from the definition of compactness that $K$ is compact.]

## A.2 Problems to Section 2

**A.2.1.** Show that if $A$ is a symmetric operator on a Hilbert space then $(\phi, A^2\phi) = (\phi, A\phi)^2$ for some unit vector $\phi \in D(A)$ if and only if $\phi$ is an eigenvector of $A$. We interpret this as saying that a measurement of $A$ in a given state $\phi$ always gives the same value if and only if $\phi$ is an eigenvector of $A$.

**A.2.2. (Some remarks on the representation (9))** In general (9) may not make sense for a general unbounded operator $A$ even if all $\psi_n \in D(A)$. For simplicity we will here consider only bounded $A$.

The general statistical average of pure states would be of the form

$$\langle A\rangle = \sum_{n=1}^{\infty} \mu_n(\phi_n, A\phi_n)$$

where $0 \leq \mu_n \leq 1$ for $n = 1, 2, \ldots$ with $\sum_{n=1}^{\infty} \mu_n = 1$ and $\phi_n$, $n = 1, 2, \ldots$ are unit vectors, but not necessarily orthonormal.

Use the result of Problem A.1.4 to show that we can find unique $0 \leq \lambda_n \leq 1$ for $n = 1, 2, \ldots$ with $\sum_{n=1}^{\infty} \lambda_n = 1$ and $\psi_n$, $n = 1, 2, \ldots$ *orthonormal* such that

$$\langle A\rangle = \sum_{n=1}^{\infty} \lambda_n(\psi_n, A\psi_n).$$

**A.2.3.** Show that the interacting Hamiltonian $H_N$ for $N$ identical Particles satisfies $H_N U_\sigma = U_\sigma H_N$ for all permutations $\sigma$. Conclude that $H_N P_\pm = P_\pm H_N$ and that $H_N$ therefore maps the subspaes $\bigwedge^N \mathfrak{h}$ and $\bigotimes_{\mathrm{SYM}}^N \mathfrak{h}$ into themselves.

## A.3 Problems to Section 3

**A.3.1.** Assume that $K$ is a positive semi-definite operator defined on a Hilbert space (full domain) such that Correction since May 3 Problem added.

$$\sum_{k=1}^{\infty} (\phi_k, K\phi_k) < \infty$$

for some orthonormal basis $\{\phi_k\}_{k=1}^{\infty}$.

(a) Use the Cauchy-Schwartz inequality for the quadratic form $Q(\phi) = (\phi, K\phi)$ to show that for all vectors $u$

$$\|Ku\|^2 \leq (Ku, u) \sum_{k=1}^{\infty} (\phi_k, K\phi_k).$$

(b) Show that $K$ is a bounded operator

(c) Use the result of Problem A.1.9 to show that $K$ is Hilbert-Schmidt

(d) Show that $K$ is trace class and that

$$\mathrm{Tr}K = \sum_{k=1}^{\infty}(\phi_k, K\phi_k).$$

## A.4 Problems to Section 4

Correction since August 30, 09: Problem added

**A.4.1.** Show that the Friedrich's extension of an operator (which is bounded below) is self-adjoint.

(Hint: the operator $B : \mathcal{H} \to D(A_F)$ defined by $(u, v)_{\mathcal{H}} = (Bu, v)_\alpha$ may be useful.)

## A.6 Problems to Section 6

**A.6.1.** Show that the molecular Hamiltonian in Example 6.5 is stable.

## A.8 Problems to Section 8

**A.8.1.** Show that for the operator $\alpha_\Psi$ defined in (41) then $\alpha_\Psi\alpha_\Psi^*$ is an trace class operator on $\mathfrak{h}$.

(Hint: use the fact $\Gamma_\Psi \geq 0$ and $\gamma_\Psi$ is of trace class.)

## A.9 Problems to Section 9

Correction since August 30, 09: Problem added

**A.9.1.** Show that the Bogolubov map $\mathcal{V}$ and the unitary implementation $\mathbb{U}_\mathcal{V}$ satisfy

$$(\mathcal{V}^*)^{-1} = (\mathcal{V}^{-1})^*, \mathbb{U}_{\mathcal{V}^{-1}} = \mathbb{U}_\mathcal{V}^{-1}.$$

Correction since August 30, 09: Problem moved from Chapter 9

**A.9.2.** Show that if $f \in \mathfrak{h}$ and $f \neq 0$ then the kernel of $a_+^*(f) + a_+(f)$ is trivial.

(Hint: Problem 9.10 may be useful. It also follows easily from Theorem 13.1.)

## A.11 Problems to Section 11

Correction since August 30, 09: Problem added

**PROBLEM A.1.** *Show that for bosons if the Hermitian, trace class operator $\mathcal{A}$ is not positive semi-definite then the quadratic Hamiltonian $H_\mathcal{A}^+$ is not bounded from below.*

**PROBLEM A.2.** *Explain why if $\mathfrak{h}$ is infinite dimensional then the method in the proof of Theorem 11.6 does not work even though in the bosonic case $\mathcal{A}$ is positive definite.*

## A.13 Problems to Section 13

Correction since August 30, 09: Problem added

**PROBLEM A.3.** *Let an infinite Hilbert space $\mathfrak{h}$ as the single particle space. For a constant $\mu > 2$ consider the Hamiltonian*

$$H = -\mu\mathcal{N} + \mathcal{N}^2$$

*on the bosonic Fock space $\mathcal{F}^B(\mathfrak{h})$ where $\mathcal{N}$ is the number operator. Define*

$$\begin{aligned} E_0 &= \inf\{(\Psi, H\Psi)|\Psi \in \mathcal{F}^B(\mathfrak{h}), ||\Psi|| = 1\}, \\ E_1 &= \inf\{(\Psi, H\Psi)|\Psi \in \mathcal{F}^B(\mathfrak{h}), \Psi \text{ is a Bogolubov variational state}\}, \\ E_2 &= \inf\{(\Psi, H\Psi)|\Psi \in \mathcal{F}^B(\mathfrak{h}), \Psi \text{ is a coherent state}\}, \\ E_3 &= \inf\{(\Psi, H\Psi)|\Psi \in \mathcal{F}^B(\mathfrak{h}), \Psi \text{ is a quasi}-\text{free pure state}\}. \end{aligned}$$

*Prove that $E_0 < E_1 < E_2 < E_3$. Moreover, $E_0, E_1, E_2$ are achieved for some ground states while $E_2$ is not achieved.*

*Here a coherent state is a state of the form $\mathbb{U}_\phi|0\rangle$ for some $\phi \in \mathfrak{h}$, where $\mathbb{U}$ is defined in Theorem 13.1. A Bogolubov variational state is a state of the form $\mathbb{U}_\phi\Psi$, where $\Psi$ is a quasi-free pure state.*

# B The Banach-Alaoglu Theorem

We shall here give a proof of the Banach-Alaoglu Theorem. It is one of the most useful tools from abstract functional analysis.

Usually this is proved using Tychonov's Theorem and thus relies on the axiom of choice. In the separable case this is however not necessary and we give a straightforward proof here.

**THEOREM B.1** (Banach-Alaoglu)**.** *Let $X$ be a Banach space and $X^*$ the dual Banach space of continuous linear functionals. Assume that the space $X$ is separable, i.e., has a countable dense subset. Then to any sequence $\{x_n^*\}$ in $X^*$ which* *is bounded, i.e., with $\|x_n^*\| \leq M$ for some $M > 0$ there exists a weak-$*$ convergent subsequence $\{x_{n_k}^*\}$ . Weak-$*$ convergent means that there exists $x^* \in X^*$ such that $x_{n_k}^*(x) \to x^*(x)$ as $k \to \infty$ for all $x \in X$. Moreover, $\|x^*\| \leq M$.*

*Proof.* Let $x_1, x_2, \ldots$ be a countable dense subset of $X$. Since $\{x_n^*\}$ is a bounded sequence we know that all the sequences

$$x_1^*(x_1), x_2^*(x_1), x_3^*(x_1), \ldots$$

$$x_1^*(x_2), x_2^*(x_2), x_3^*(x_2), \ldots$$

$$\vdots$$

are bounded. We can therefore find convergent subsequences

$$x_{n_{11}}^*(x_1), x_{n_{12}}^*(x_1), x_{n_{13}}^*(x_1) \ldots$$

$$x_{n_{21}}^*(x_2), x_{n_{22}}^*(x_2), x_{n_{23}}^*(x_2) \ldots$$

$$\vdots$$

with the property that the sequence $n_{(k+1)1}, n_{(k+1)2}, \ldots$, is a a subsequence of $n_{k1}, n_{k2}, \ldots$. It is then clear that the tail $n_{kk}, n_{(k+1)(k+1)}, \ldots$ of the diagonal sequence $n_{11}, n_{22}, \ldots$ is a subsequence of $n_{k1}, n_{k2}, \ldots$ and hence that for all $k \geq 1$ the sequence

$$x_{n_{11}}^*(x_k), x_{n_{22}}^*(x_k), x_{n_{33}}^*(x_k) \ldots$$

is convergent. Now let $x \in X$ be any element of the Banach space then

$$\begin{aligned} |x_{n_{pp}}^*(x) - x_{n_{qq}}^*(x)| &\leq |x_{n_{pp}}^*(x) - x_{n_{pp}}^*(x_k)| + |x_{n_{qq}}^*(x) - x_{n_{qq}}^*(x_k)| \\ &\quad + |x_{n_{pp}}^*(x_k) - x_{n_{qq}}^*(x_k)| \\ &\leq 2M\|x - x_k\| + |x_{n_{pp}}^*(x_k) - x_{n_{qq}}^*(x_k)|. \end{aligned}$$

Since $\{x_k\}$ is dense we conclude that $x_{n_{pp}}^*(x)$ is a Cauchy sequence for all $x \in X$. Hence $x_{n_{pp}}^*(x)$ is a convergent sequence for all $x \in X$. Define $x^*$ by $x^*(x) = \lim_{p\to\infty} x_{n_{pp}}^*(x)$. Then $x^*$ is clearly a linear map and $|x^*(x)| \leq M\|x\|$. Hence $x^* \in X^*$ and $\|x^*\| \leq M$. $\square$

**COROLLARY B.2** (Banach-Alaoglu on Hilbert spaces)**.** *If $\{x_n\}$ is a bounded sequence in a Hilbert space $\mathcal{H}$ (separable or not) then there exists a subsequence $\{x_{n_k}\}$ that converges weakly in $\mathcal{H}$ to an element $x \in \mathcal{H}$ with $\|x\| \leq \liminf_{n\to\infty} \|x_n\|$.*

*Proof.* Consider the space $X$ which is the closure of the space spanned by $x_n$, $n = 1, 2, \ldots$. This space $X$ is a separable Hilbert space and hence is its own dual. Thus we may find a subsequence $\{x_{n_k}\}$ and an $x \in X$ such that $x_{n_k} \to x$ weakly in $X$. If $y \in \mathcal{H}$ let $y'$ be its orthogonal projection onto $X$. We then have

$$\lim_k (x_{n_k}, y) = \lim_n (x_n, y') = (x, y') = (x, y).$$

Thus $x_{n_k} \to x$ weakly in $\mathcal{H}$. □

# C Proof of the min-max principle

In this section we give the proof of Theorem 4.12.

The operator $A$ is bounded from below, i.e., $A \geq -\alpha I$. In fact, from (13) we may choose $\alpha = -\mu_1$. We first note that since vectors in $D(Q)$ may be approximated in the $\|\cdot\|_\alpha$ norm by vectors in $D(A)$ we may write

$$\mu_n = \mu_n(A) = \inf\left\{ \max_{\phi \in M,\ \|\phi\|=1} Q(\phi) \ :\ M \subseteq D(Q), \quad \dim M = n \right\}.$$

In particular, it is no loss of generality to assume that $A$ is already the Friederichs' extension. It is clear that the sequence $(\mu_n)$ is non-decreasing.

We shall prove several intermediate results, which we formulate as lemmas.

**LEMMA C.1.** *If for some $m \geq 1$ we have $\mu_m < \mu_{m+1}$ then $\mu_1$ is an eigenvalue of $A$.*

*Proof.* Our aim is to prove that there is a unit vectors $\psi \in D(Q)$ such that $Q(\psi) = \mu_1$. It then follows from Problem 3.10 that $\psi$ is an eigenfunction of $A$ with eigenvalue $\mu_1$.

We may assume that $\mu_1 = \mu_m < \mu_{m+1}$. We choose a sequence $(M_n)$ of $m$-dimensional spaces such that

$$\max_{\phi \in M_n,\ \|\phi\|=1} Q(\phi) \leq \mu_1 + 2^{-4-n}(\mu_{m+1} - \mu_1).$$

We claim that we can find a sequence of unit vectors $\psi_n \in M_n$, $n = 1, 2, \ldots$ such that

$$\|\psi_n - \psi_{n+1}\| \leq 2^{-n}. \tag{86}$$

In particular, the sequence is Cauchy for the norm $\|\cdot\|$. We choose $\psi_n$ inductively. First $\psi_1 \in M_1$ is chosen randomly. Assume we have chosen $\psi_n \in M_n$. If $\psi_n \in M_{n+1}$ we simply choose $\psi_{n+1} = \psi_n$. Otherwise $\dim \mathrm{span}(\{\psi_n\} \cup M_{n+1}) = m+1$ and hence we can find a unit vector $\widetilde{\psi} \in \mathrm{span}(\{\psi_n\} \cup M_{n+1})$ such that $Q(\widetilde{\psi}) \geq \mu_{m+1}$. In particular, we cannot have $\widetilde{\psi} \in M_n$ or $\widetilde{\psi} \in M_{n+1}$. We may write $\widetilde{\psi} = u_1 - u_2$, where $u_1 = \lambda\psi_n$, $\lambda \neq 0$ and $u_2 \in M_{n+1} \setminus \{0\}$. We therefore have

Corrections since August 30, 09: $\mathrm{span}(\{\psi_{n+1}\} \cup M_{n+1}) \to \mathrm{span}(\{\psi_n\} \cup M_{n+1})$; "$u_1 = \lambda\psi_1$" $\to$ "$u_1 = \lambda\psi_n$".

$$\begin{aligned}
\mu_{m+1} &\leq Q(u_1 - u_2) = 2Q(u_1) + 2Q(u_2) - Q(u_1 + u_2) \\
&\leq 2(\mu_1 + 2^{-4-n}(\mu_{m+1} - \mu_1))(\|u_1\|^2 + \|u_2\|^2) - Q(u_1 + u_2) \\
&\leq 2(\mu_1 + 2^{-4-n}(\mu_{m+1} - \mu_1))(\|u_1\|^2 + \|u_2\|^2) - \mu_1\|u_1 + u_2\|^2 \\
&= \mu_1\|u_1 - u_2\|^2 + 2^{-3-n}(\mu_{m+1} - \mu_1)(\|u_1\|^2 + \|u_2\|^2) \\
&= \mu_1 + 2^{-3-n}(\mu_{m+1} - \mu_1)(\|u_1\|^2 + \|u_2\|^2)
\end{aligned}$$

where the last inequality follows since $Q(\phi) \geq \mu_1\|\phi\|^2$ for all $\psi \in D(Q)$. We can rewrite this as

$$2^{n+3} \leq \|u_1\|^2 + \|u_2\|^2. \tag{87}$$

Since both $u_1, u_2$ are non-zero we may use the geometric inequality

$$\left\| \frac{u_1}{\|u_1\|} - \frac{u_2}{\|u_2\|} \right\| \leq 2\frac{\|u_1 - u_2\|}{\max\{\|u_1\|, \|u_2\|\}}.$$

Combining this with (87) and recalling that $\|u_1 - u_2\| = 1$ we obtain

$$\left\| \frac{u_1}{\|u_1\|} - \frac{u_2}{\|u_2\|} \right\|^2 \leq \frac{8}{\|u_1\|^2 + \|u_2\|^2} \leq 2^{-n}$$

and (86) follows with $\psi_n = u_2/\|u_2\|$.

Corrections since August 30, 09: $\psi_2 \to \psi_n$.

Since $(\psi_n)$ is Cauchy for the norm $\|\cdot\|$ we have $\psi \in \mathcal{H}$ such that $\psi_n \to \psi$ for $n \to \infty$ . In particular, $\psi$ is a unit vector. We will now prove that $\psi \in D(Q)$ and that $Q(\psi) = \mu_1$ thus establishing the claim of the lemma.

Since $Q(\psi_n) \to \mu_1$ as $n \to \infty$ we have that

$$\|\psi_n\|_\alpha^2 = (\alpha + 1) + Q(\psi_n) \to \alpha + 1 + \mu_1$$

as $n \to \infty$. In particular, $\|\psi_n\|_\alpha$ is bounded. Since $D(Q)$ is a Hilbert space with the inner product

$$(\phi_1, \phi_2)_\alpha = (\alpha + 1)(\phi_1, \phi_2) + Q(\phi_1, \phi_2)$$

we conclude from the Banach-Alaoglu Theorem for Hilbert spaces Corollary B.2 that there is a subsequence $(\psi_{n_k})$ that converges weakly in $D(Q)$ to some $\psi' \in D(Q)$. We must have $\psi = \psi'$. In fact, for all $\phi \in \mathcal{H}$ we have a continuous linear functional on $D(Q)$ given by $D(Q) \ni u \mapsto (\phi, u) \in \mathbb{C}$. Simply note that $|(\phi, u)| \leq \|\phi\|\|u\| \leq \|\phi\|\|u\|_\alpha$. Thus for all $\phi \in \mathcal{H}$ we have

$$(\phi, \psi') = \lim_{k\to\infty} (\phi, \psi_{n_k}) = (\phi, \psi).$$

Hence $\psi \in D(Q)$. We also have that

$$\|\psi\|_\alpha^2 = \lim_{k\to\infty} (\psi, \psi_{n_k})_\alpha \leq \|\psi\|_\alpha \lim_{k\to\infty} \|\psi_{n_k}\|_\alpha$$

and thus

$$\|\psi\|_\alpha \leq \lim_{k\to\infty} \|\psi_{n_k}\|_\alpha = \alpha + 1 + \mu_1.$$

Therefore

$$Q(\psi) = \|\psi\|_\alpha^2 - (\alpha + 1)\|\psi\|^2 = \|\psi\|_\alpha^2 - (\alpha + 1) \leq \mu_1.$$

Since the opposite inequality $Q(\psi) \geq \mu_1$ holds for all unit vectors in $D(Q)$ we finally conclude that $Q(\psi) = \mu_1$. □

By induction on $k$ we will show that if $\mu_K < \mu_{K+1}$ for some $K \geq k$ then $\mu_1, \ldots, \mu_k$ are eigenvalues for $A$ counted with multiplicities. If $k = 1$ this is simply Lemma C.1. Assume the result has been proved for $k \geq 1$ and that $\mu_K < \mu_{K+1}$ for some $K \geq k + 1$. By the induction assumption we know that $\mu_1, \ldots, \mu_k$ are eigenvalues for $A$ counted with multiplicities. Let $\phi_1, \ldots, \phi_k$ be corresponding orthonormal eigenvectors. Consider the space

$$V_k = \text{span}\{\phi_1, \ldots, \phi_k\}^\perp.$$

Since $A$ is symmetric it will map $V_k \cap D(A)$ into $V_k$ and the restriction $A_k$ of $A$ to $V_k \cap D(A)$ is the operator corresponding to the restriction $Q_k$ of the quadratic form $Q$ to $V_k \cap D(Q)$.

That $\mu_{k+1}$ is an eigenvalue of $A_k$ and hence an additional eigenvalue of $A$ (counted with mulitplicity) follows from Lemma C.1 and the following claim.

**LEMMA C.2.**

$$\mu_n(A_k) = \mu_{n+k}(A).$$

*Proof.* If $M$ is any $n+k$-dimensional subspace of $D(Q)$ then the projection of $\mathrm{span}\{\phi_1,\ldots,\phi_k\}$ onto $M$ is at most $k$-dimensional and hence $M\cap V_k$ must have dimension at least $n$. Thus

$$\max_{\phi\in M,\ \|\phi\|=1} Q(\phi) \geq \max_{\phi\in M\cap V_k,\ \|\phi\|=1} Q(\phi) \geq \mu_n(A_k).$$

Thus

$$\mu_{k+n}(A) \geq \mu_n(A_k).$$

To prove the opposite inequality note that if $\phi=\phi_1+\phi_2\in D(Q)$ with $\phi_1\in V_k$ and $\phi_2\in\mathrm{span}\{\phi_1,\ldots,\phi_k\}$ we have

$$Q(\phi) = Q(\phi_1)+Q(\phi_2). \tag{88}$$

We first show that $\mu_1(A_k)\geq\mu_k(A)$. Assume otherwise that $\mu_1(A_k)<\mu_k(A)$ we can then find a unit vector $\phi'\in V_k$ such that $Q(\phi')<\mu_k(A)$. Let $j$ be the largest integer such that $\mu_j(A)\leq\mu_1(A_k)$ (this is certainly true for $j=1$). Then $j<k$. If we consider the $j+1$-dimensional space $M=\mathrm{span}\{\phi_1,\ldots,\phi_j,\phi'\}$ we see from (88) that

$$\mu_{j+1}(A) \leq \max_{\phi\in M,\ \|\phi\|=1} Q(\phi) \leq \mu_1(A_k)$$

which contradicts the fact that $j$ was the largest integer with this property. Hence we must have $\mu_1(A_k)\geq\mu_k(A)$.

From (88) we find that if $M'$ is any $n$-dimensional subspace of $V_k$ for $n\geq 0$ we have for the $n+k$-dimensional subspace $M=M'\oplus\mathrm{span}\{\phi_1,\ldots,\phi_k\}$ that

$$\max_{\phi\in M,\ \|\phi\|=1} Q(\phi) = \max\left\{\mu_k(A), \max_{\phi\in M',\ \|\phi\|=1} Q(\phi)\right\}.$$

Hence

$$\mu_{k+n}(A) \leq \max\{\mu_k(A),\mu_n(A_k)\} = \mu_n(A_k).$$

□

The statement in the second paragraph of Theorem 4.12 follows immediately from Lemma C.2. The last statement is an easy exercise left for the reader.

# D Analysis of the function $\mathcal{G}(\lambda, Y)$ in (37)

If we use the inequality $2ab \leq a^2 + b^2$ on the last term in $\mathcal{G}(\lambda, Y)$ we see that

$$\begin{aligned}\mathcal{G}(\lambda, Y) \;\leq\; & \frac{(1-\lambda^2)\,(1-Y^2)\,N\,(M-N)}{M-2} + \frac{(1-\lambda^2)\,Y^2\,(N-2)\,(M-N+2)}{M-2} \\ & +2\,\lambda^2 Y^2 + 2\,Y^2\left(1-Y^2\right) + \frac{\lambda^2\,(1-\lambda^2)\,(M-N)\,N}{M-2}.\end{aligned}$$

We see that this expression is a quadratic polynomial $p(x,y)$ in the variables $x = \lambda^2$, $y = Y^2$. Straightforward calculations show that

$$\frac{\partial^2}{\partial x^2} p(x,y) = -2\,\frac{N\,(M-N)}{M-2},\;\; \frac{\partial^2}{\partial y^2} p(x,y) = -4,\;\; \frac{\partial^2}{\partial x \partial y} p(x,y) = 4\,\frac{M-N}{M-2}$$

and that

$$\frac{\partial}{\partial x} p(x,y)(2/M, N/M) = 0, \quad \frac{\partial}{\partial y} p(x,y)(2/M, N/M) = 0.$$

In particular,

$$\frac{\partial^2 p}{\partial x^2}\frac{\partial^2 p}{\partial y^2} - \left(\frac{\partial^2 p}{\partial x \partial y}\right)^2 = 8\,\frac{(M-N)\,M\,(N-2)}{(M-2)^2} \geq 0.$$

This shows (by the second derivative test) that $p(x,y)$ is maximal for $(x,y) = (2/M, N/M)$. Thus

$$\mathcal{G}(\lambda, Y) \leq p(2/M, N/M) = \frac{N(M-N+2)}{M} = \mathcal{G}((2/M)^{1/2}, (N/M)^{1/2}).$$

# E Results on conjugate linear maps

Recall that a conjugate linear map $C : \mathcal{H} \to \mathcal{K}$ between complex vector spaces $\mathcal{H}$ and $\mathcal{K}$ is a map such that

$$C(\alpha u + \beta v) = \overline{\alpha} C(u) + \overline{\beta} C(v)$$

for all $u, v \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{C}$.

We will concentrate on the situation where $\mathcal{H}$ and $\mathcal{K}$ are Hilbert spaces.

The map $J : \mathcal{H} \to \mathcal{H}^*$ given by $J(\phi)(\psi) = (\phi, \psi)$ (see also Remark 1.2) is conjugate linear.

The adjoint of a conjugate linear map $C : \mathcal{H} \to \mathcal{K}$ is the conjugate linear map $C^* : \mathcal{K} \to \mathcal{H}$ defined by

$$(Ch, k)_{\mathcal{K}} = (C^*k, h)_{\mathcal{H}}, \quad \text{for all } h \in \mathcal{H}, k \in \mathcal{K} \tag{89}$$

The map $J : \mathcal{H} \to \mathcal{H}^*$ is anti-unitary meaning

$$J^*J = I_{\mathcal{H}} \quad \text{and} \quad JJ^* = I_{\mathcal{H}^*}. \tag{90}$$

**PROBLEM E.1.** *Show that (89), indeed, defines a conjugate linear map $C^*$ and show the identities in (90).*

**THEOREM E.2** (Conjugate Hermitian and anti-Hermitian maps)**.**
*Let $C : \mathcal{H} \to \mathcal{H}$ be a conjugate linear map such that $C^*C$ admits an orthonormal eigenbasis. If $C : \mathcal{H} \to \mathcal{H}$ is a conjugate Hermitian map, i.e., a conjugate linear map satisfying $C^* = C$ then $\mathcal{H}$ has an orthonormal basis of eigenvectors for $C$ and all the eigenvalues are non-negative (in particular real).*

Correction since August 30, 09: Condition on $C^*C$ reformulated for non-compact operators

*If $C : \mathcal{H} \to \mathcal{H}$ is conjugate anti-Hermitian, i.e., a conjugate linear map satisfying $C^* = -C$ then ker$(C)$ is a closed subspace of $\mathcal{H}$ and the space ker$(C)^\perp$ has an orthonormal basis*

$$u_1, u_2 \ldots$$

*such that*

$$Cu_{2i} = \lambda_i u_{2i-1},\ Cu_{2i-1} = -\lambda_i u_{2i},$$

*where $\lambda_i > 0$, $i = 1, 2, \ldots$.*

The condition that $C^*C$ can be diagonalized holds if, for example, $C^*C$ is trace class or $C$ is anti-unitary.

*Proof.* The operator $C^*C$ is a *linear* Hermitian positive semi-definite map since $(C^*Cu, u) = (Cu, Cu) \geq 0$. Therefore its eigenvalue must be non-negative (in particular real). Moreover, if $C$ is Hermitian or anti-Hermitian $C$ maps the eigenspace of $C^*C$ into itself. Assume that $u$ is a normalized eigenvector for $C^*C$, i.e.,

Correction since June 24: Invariance of eigenspaces under $C$ added

$$C^*Cu = \lambda^2 u$$

for some $\lambda \geq 0$.

Correction since June 24: $u, w$ in eigenspace of $C^*C$ added

We consider first the case $C^* = C$. We then have $(C+\lambda)(C-\lambda)u = (C^2 - \lambda^2)u = 0$. Hence either $(C-\lambda)u = 0$ or $w = (C-\lambda)u \neq 0$ and $(C+\lambda)w = 0$. We have thus found one eigenvector (either $u$ or $w$) for $C$, which belong to the eigenspace of $C^*C$ with eigenvalue $\lambda$. We can always assume the eigenvalue is non-negative by eventually multiplying the eigenvector by $i$ and using the conjugate linearity, i.e., $Ciw = -iCw = \lambda iw$ if $Cw = -\lambda w$. We may show that $C$ maps the orthogonal complement of this eigenvector into itself and then finish the proof by an induction which is left as an exercise for the reader.

Correction since August 30, 09: The restricted problem in the orthogonal complement is formulated as an exercise.

Consider next the case when $C^* = -C$. If the eigenvalue $\lambda^2$ of $C^*C$ vanishes then $Cu = 0$, since $(Cu, Cu) = (C^*Cu, u) = 0$. We can therefore choose $u$ as one of the basis vectors. We may then proceed as before and show that $C$ maps the orthogonal complement of $u$ into itself and then reduce the problem to a space of lower dimension.

If $\lambda > 0$ then $\|Cu\| = \lambda$ and we define the unit vector $w = \lambda^{-1}Cu$. Then $Cu = \lambda w$ and

$$Cw = \lambda^{-1}C^2u = -\lambda^{-1}C^*Cu = -\lambda^{1}\lambda^2 u = -\lambda u.$$

Moreover,

$$(w, u) = \lambda^{-1}(Cu, u) = \lambda^{-1}(C^*u, u) = -\lambda(Cu, u) = -(w, u).$$

Thus $(w, u) = 0$. Thus $u$ and $w$ can be the first two vectors in the orthonormal basis.

We then can show that $C$ maps the orthogonal complement of $\{u, w\}$ into itself and finish the proof by induction. □

**PROBLEM E.3.** *Assume that $f : \mathcal{H} \to \mathcal{H}$ is Hermitian or conjugate Hermitian or conjugate anti-Hermitian. Let $X$ be a closed subspace of $\mathcal{H}$ such that $f$ leaves $X$ invariant. Prove that $f$ leaves $X^\perp$ invariant. Moreover, show that if $f$ has an eigenvector $u \in \mathcal{H}\backslash X$ then $f$ also has an eigenvector $v \in X^\perp$ such that $u \in \mathrm{Span}(X \cup \{v\})$.*

*Proof of Lemma 8.14.* To each element $f \in \mathfrak{h} \wedge \mathfrak{h}$ we may associate a conjugate linear map $C_f : \mathfrak{h} \to \mathfrak{h}$ by

$$(\phi, C_f\psi)_{\mathfrak{h}} = (\phi \wedge \psi, f)_{\mathfrak{h}\wedge\mathfrak{h}}$$

for all $\phi, \psi \in \mathfrak{h}$. Then

$$(\phi, C_f^* \psi)_{\mathfrak{h}} = (\psi, C_f \phi)_{\mathfrak{h}} = (\psi \wedge \phi, f)_{\mathfrak{h}\wedge\mathfrak{h}} = -(\phi, C_f \psi)_{\mathfrak{h}}.$$

Hence $C_f$ is a conjugate anti-Hermitian map. We may then choose an orthonormal basis $u_1, \ldots, u_{2r}, u_{2r+1}, \ldots, u_M$ for $\mathfrak{h}$ such that $u_{2r+1}, \ldots, u_M$ are in the kernel of $C_f$ and $u_1, \ldots, u_{2r}$ are as described in Theorem E.2. We claim that

$$f = \sum_{i=1}^{r} \lambda_i u_{2i-1} \wedge u_{2i}.$$

This follows from

$$\begin{aligned}
(\phi \wedge \psi, f) &= (\phi, C_f \psi) = \sum_{i=1}^{n} \sum_{j=1}^{n} (\phi, u_i)(u_i, C_f (u_j, \psi) u_j) \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} (\phi, u_i)(u_i, C_f u_j)(\psi, u_j) \\
&= \sum_{i=1}^{r} (\phi, u_{2i-1})(u_{2i-1}, C_f u_{2i})(\psi, u_{2i}) + (\phi, u_{2i})(u_{2i}, C_f u_{2i-1})(\psi, u_{2i-1}) \\
&= \sum_{i=1}^{r} \lambda_i ((\phi, u_{2i-1})(\psi, u_{2i}) - (\phi, u_{2i})(\psi, u_{2i-1})) \\
&= (\phi \wedge \psi, \sum_{i=1}^{r} \lambda_i u_{2i-1} \wedge u_{2i}).
\end{aligned}$$

□

# F The necessity of the Shale-Stinespring condition

Correction since August 30, 09: Proof added

Assume that there exists a normalized vector $|0\rangle_{\mathcal{V}}$ in $\mathcal{F}^{B,F}(\mathfrak{h})$ such that

$$A_{\pm}(\mathcal{V}(u \oplus 0))\,|0\rangle_{\mathcal{V}} = 0, \quad \forall u \in \mathfrak{h}. \tag{91}$$

We need to prove that $V^*V$ must be trace class. [17].

[17]The proof follows ideas of Ruijsenaars S.N.M, On Bogoliubov transformations for systems of relativistic charged particles, J. Math. Phys., Vol. 18, No. 3 (1977) - Theorem 6.1.

*Proof.* Denote $|0\rangle_{\mathcal{V}} = \bigoplus_{N=0}^{\infty} \Psi_N$. Then (91) is equivalent to

$$a_\pm(Uu)\Psi_1 = 0, \quad a_\pm(Uu)\Psi_{N+2} + a_\pm^*(J^*Vu)\Psi_N = 0, \quad \forall u \in \mathfrak{h}, N = 0, 1, 2, ... \quad (92)$$

We first consider the bosonic case. We claim that $\Psi_0 \neq 0$. From (58) we have $U^*$ is injective and hence $\overline{\mathrm{Ran}(U)} = \mathfrak{h}$. Thus (92) implies $\Psi_1 = \Psi_3 = \Psi_5 = ... = 0$. If $\Psi_0 = 0$ then $\Psi_0 = \Psi_2 = \Psi_4 = ... = 0$ which contradicts with $|0\rangle_{\mathcal{V}} \neq 0$. Thus $\Psi_0 \in \mathbb{C}\backslash\{0\}$. In particular, we deduce from (92) that

$$J^*Vu = -\Psi_0^{-1} a_+(Uu)\Psi_2, \quad \forall u \in \mathfrak{h}. \quad (93)$$

Introducing a conjugate linear map $H_B : \mathfrak{h} \to \mathfrak{h}$ defined by

$$(H_B\varphi_1, \varphi_2) = (\Psi_2, \varphi_1 \otimes \varphi_2), \quad \forall \varphi_1, \varphi_2 \in \mathfrak{h}.$$

It is straightforward to check that $H_B^* H_B$ is trace class (here we do not need the symmetry of $\Psi_2$) and

$$\mathrm{Tr}(H_B^* H_B) = \|\Psi_2\|^2 .$$

Moreover using (93) and the symmetry of $\Psi_2$ we have

$$J^*V = -\sqrt{2}\Psi_0^{-1} H_B U$$

since

$$\begin{aligned}(-\Psi_0 J^*V\varphi_1, \varphi_2) &= (a_+(U\varphi_1)\Psi_2, \varphi_2) = (\Psi_2, a_+^*(U\varphi_1)\varphi_2,) \\ &= \sqrt{2}(\Psi_2, U\varphi_1 \otimes U\varphi_2) = \sqrt{2}(H_B U\varphi_1, \varphi_2)\end{aligned}$$

for all $\varphi_1, \varphi_2 \in \mathfrak{h}$. Thus

$$V^*V = 2\Psi_0^{-2} U^* H_B^* H_B U$$

is indeed a trace class map on $\mathfrak{h}$.

We now turn to the fermionic case. This case is a little more complicated because $U^*$ is not necessary to be injective and we can not conclude $\Psi_0 \neq 0$. Let $u_1, u_2, ...$ be an orthonormal basis for $\mathfrak{h}$ such that $u_i \in \mathrm{Ker}(U^*)$ if $i \in K \subset \mathbb{N}$ and $u_i \in \mathrm{Ran}(U)$ if $i \in \mathbb{N}\backslash K$.

We claim that $\dim\mathrm{Ker}(U^*)) = L < \infty$ and if $\mathrm{Span}\{u_1, ..., u_L\} = \mathrm{Span}(U^*)$ then

$$\begin{aligned}\Psi_N &= 0 \text{ if } N < L, &(94)\\ \Psi_N &= P_-(\Lambda_N \otimes (u_1 \wedge ... \wedge u_L)) \text{ with } \Lambda_N \in \bigwedge^{N-L} \overline{\mathrm{Ran}(U)} \text{ if } N \geq L. &(95)\end{aligned}$$

Indeed, using (68) and (92) we have

$$a_-^*(u)\Psi_N = 0, \quad \forall u \in \mathrm{Ker}(U^*), N = 0, 1, 2, ...$$

Each $\Psi_N$ can be expressed by

$$\Psi_M = \sum_{1 \le i_1 < ... < i_N} \alpha_{i_1,...,i_N} u_{i_1} \wedge ... \wedge u_{i_N}, \quad \alpha_{i_1,...,i_N} \in \mathbb{C}.$$

Note that $a_-^*(u_j)u_{i_1} \wedge ... \wedge u_{i_N} = 0$ if and only if $j \in \{i_1, ..., i_N\}$. Thus

$$\mathrm{K} \subset \{i_1, ..., i_N\} \quad \text{if} \quad \alpha_{i_1,...,i_N} \neq 0. \tag{96}$$

In particular, denote $L = |K|$ then $L \le N$ if $\Psi_N \neq 0$. Because $|0\rangle_{\mathcal{V}} \neq 0$ we must have $\Psi_N \neq 0$ for some $N$ and hence dim $\mathrm{Ker}(U^*) = L < \infty$. We of course can assume that $\mathrm{K} = \{1, ..., L\}$, i.e. $\mathrm{Span}\{u_1, ..., u_L\} = \mathrm{Ker}(U^*)$, and (94)-(95) easily follows from (96).

We now prove $\Psi_L \neq 0$. Because (94), it follows from (92) that $a_-(Uu)\Psi_{L+1} = 0$ for all $u \in \mathfrak{h}$. Using (95) and $\mathrm{Ker}(U^*) = \mathrm{Ran}(U)^\perp$ we have

$$a_-(Uu)\Psi_N = c_{N,L} P_-((a_-(Uu)\Lambda_N) \otimes (u_1 \wedge ... \wedge u_L)), \quad \forall N \ge L, \tag{97}$$

where $c_{N,L} \in \mathbb{R}\backslash\{0\}$. Therefore $a_-(Uu)\Psi_{L+1} = 0$ implies $a_-(Uu)\Lambda_{L+1} = 0$ for all $u \in \mathfrak{h}$. Because $\Lambda_{L+1} \in \overline{\mathrm{Ran}(U)}$ we deduce that $\Lambda_{L+1} = 0$, and consequently $\Psi_{L+1} = 0$. Using (92) repeatedly we get $\Psi_{L+1} = \Psi_{L+3} = \Psi_{L+5} = ... = 0$. If $\Psi_L = 0$ then the same argument implies that $\Psi_L = \Psi_{L+2} = \Psi_{L+4} = ... = 0$ which contradicts with $|0\rangle_{\mathcal{V}} \neq 0$. Thus $\Psi_L \neq 0$.

We now can process similarly to the bosonic case in which $(\Lambda_{L+2}, \overline{\mathrm{Ran}(U)})$ replaces $(\Psi_2, \mathfrak{h})$. More precisely, we define a conjugate linear map $H_F : \overline{\mathrm{Ran}(U)} \to \overline{\mathrm{Ran}(U)}$ by

$$(H_F\varphi_1, \varphi_2) = (\Lambda_{L+2}, \varphi_1 \otimes \varphi_2), \quad \forall \varphi_1, \varphi_2 \in \overline{\mathrm{Ran}(U)}.$$

Then $H_F^* H_F$ is a trace class map on $\overline{\mathrm{Ran}(U)}$. Moreover it is straightforward to check that $J^*V = -\beta H_F U$ on $\overline{\mathrm{Ran}(U)}$ for some $\beta \in \mathbb{R}\backslash\{0\}$. Indeed, recall that $\Psi_L = \Lambda_L u_1 \wedge ... \wedge u_L$ and $\mathrm{Ker}(U^*) = \mathrm{Ran}(U)^\perp$. Using (92) and (97) we have

$$(-J^*V\varphi_1, \varphi_2) \;\; = \;\; L!\sqrt{L+1}\Lambda_L^{-2}(-a_-^*(J^*V\varphi_1)\Psi_L, \varphi_2 \otimes \Psi_L)$$

$$
\begin{aligned}
&= L!\sqrt{L+1}\Lambda_L^{-2}(a_-(U\varphi_1)\Psi_{L+2}, \varphi_2 \otimes \Psi_L) \\
&= L!\sqrt{L+1}\Lambda_L^{-3}c_{L+2,L}(P_-(a_-(U\varphi_1)\Lambda_{L+2}) \otimes \Psi_L), \varphi_2 \otimes \Psi_L) \\
&= (L+1)^{-1/2}\Lambda_L^{-1}c_{L+2,L}(a_-(U\varphi_1)\Lambda_{L+2}, \varphi_2) \\
&= (L+1)^{-1/2}\Lambda_L^{-1}c_{L+2,L}(\Lambda_{L+2}, a_-^*(U\varphi_1)\varphi_2) \\
&= \beta(\Lambda_{L+2}, U\varphi_1 \otimes \varphi_2) = \beta(H_F U\varphi_1, \varphi_2)
\end{aligned}
$$

for all $\varphi_1, \varphi_2 \in \overline{\mathrm{Ran}(U)}$. Thus $V^*V = \beta^2 U^* H_F^* H_F U$ is a trace class operator on $\overline{\mathrm{Ran}(U)}$. Because $\mathrm{Ker}(U^*)$ is finite dimensional, we conclude that

$$V^*V = V^*V \circ \mathrm{Proj}_{\overline{\mathrm{Ran}(U)}} + V^*V \circ \mathrm{Proj}_{\mathrm{Ker}(U^*)}$$

is indeed a trace class map on $\mathfrak{h}$. □

# G Generalized one-particle density matrices of quasi-free states

Correction since August 30, 09: Section added

The generalized 1-pdm defined for pure states in Section 8.2 may be extended for quantum mechanical state. Recall that a quantum state $\rho$ may be considered as a complex-valued linear map acting on the set of operators of the Fock space $\mathcal{F}^{B,F}(\mathfrak{h})$ such that

$$\rho[B] = \mathrm{Tr}(BP)$$

for all linear bounded operator $B$, where $P$ is a positive semi-definite trace class operator with $\mathrm{Tr}(P) = 1$. In particular, a normalized pure state $\Psi \in \mathcal{F}^{B,F}(\mathfrak{h})$ may be considered as a quantum state $\rho$ with $P = P_\Psi$, the orthogonal projection onto $\mathrm{Span}\{\Psi\}$.

From the physical motivation we are mainly interested in quantum states with finite particle expectation, i.e. $\rho[\mathcal{N}] < \infty$.

**DEFINITION G.1** (1-pdm of quantum states)**.** Let $\rho$ be a quantum state with finite particle expectation. The corresponding one-particle density matrix $\Gamma$ is a linear operator on $\mathfrak{h} \oplus \mathfrak{h}^*$ defined by

$$(F_1, \Gamma F_2) = \rho[A^*(F_2)A(F_1)] \quad \text{for all } F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}^*.$$

Similarly to 1-pdm of pure states, the 1-pdm $\Gamma$ of a quantum state may be written in the block form

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \pm J\alpha J & 1 \pm J\gamma J^* \end{pmatrix} \tag{98}$$

with (+) for bosons and (-) for fermions, where $\gamma : \mathfrak{h} \to \mathfrak{h}$ and $\alpha : \mathfrak{h}^* \to \mathfrak{h}$ are linear operators.

We shall restrict our consideration on the class of *quasi-free states*, the quantum states satisfy Wick's Theorem, i.e.

$$\begin{aligned} &\rho[A_\pm(F_1)...A_\pm(F_{2m})] \\ &\quad = \sum_{\sigma \in P_{2m}} (\pm 1)^\sigma \rho[A_\pm(F_{\sigma(1)})A_\pm(F_{\sigma(2)})]...\rho[A_\pm(F_{\sigma(2m-1)})A_\pm(F_{\sigma(2m)})] \end{aligned} \tag{99}$$

and

$$\rho[A_\pm(F_1)...A_\pm(F_{2m-1})] = 0. \tag{100}$$

for all $m \geq 1$ (see also (75) and (76)).

The point is that a quasi-free state is determined uniquely by its 1-pdm. Moreover, the class of 1-pdm of quasi-free states is invariant under Bogolubov transformation.

**PROBLEM G.2** (Action of Bogolubov maps on 1-pdm of quasi-free states)**.** *Let $\Gamma$ be the 1-pdm of a quasi-free state $\rho$. Let $\mathcal{V}$ be a Bogolubov map which admits a unitary implementation $\mathbb{U}_\mathcal{V}$. Prove that $\mathcal{V}^*\Gamma\mathcal{V}$ is the 1-pdm of the quasi-free state $\rho'$ defined by*

$$\rho'[B] = \rho[\mathbb{U}_\mathcal{V} B \mathbb{U}_\mathcal{V}^*].$$

We now consider the structure of quasi-free states.

**THEOREM G.3.** *Let $\{u_n\}_{n=1}^\infty$ be an orthogonal basis for $\mathfrak{h}$. For a subset $I \subset \mathbb{N}$ let $\lambda_n > 0$ such that $\sum_{n \in I} e^{-\lambda_n} < \infty$. Let*

$$G = \Pi_0 \exp\left[ -\sum_{n \in I} \lambda_n a_\pm^*(u_n) a_\pm(u_n) \right]$$

*where* $\Pi_0$ *is the projection onto the subspace* $\mathrm{Ker}[\sum_{n\notin I} a_\pm^*(u_n)a_\pm(u_n)]$. *Then* $G$ *is a trace class operator on the Fock space* $\mathcal{F}^{B,F}(\mathfrak{h})$ *and the state* $\rho$ *defined by*

$$\rho[B] = \frac{\mathrm{Tr}[BG]}{\mathrm{Tr}[G]}$$

*is a quasi-free state.*

The subspace $\mathrm{Ker}[\sum_{n\notin I} a_\pm^*(u_n)a_\pm(u_n)]$ consists of all pure states without particles $\{u_n\}_{n\notin I}$. In other words it is the Fock space associated with the Hilbert space spaned by $\{u_n\}_{n\in I}$. If $I=\emptyset$ then $\rho$ is just the vacuum while if $I=\mathbb{N}$ then $\rho$ is a Gibbs state.

*Proof.* We shall prove for the bosons and the fermions is similar. We first consider the case $I=\mathbb{N}$. We want to check that $G$ is trace class. Denote $a_i = a_+(u_i)$ for short. Recall that an orthonormal basis of $\mathcal{F}^B(\mathfrak{h})$ is given by

$$|n_1,n_2,...\rangle = (n_1!n_2!...)^{-1/2}(a_1^*)^{n_1}(a_2^*)^{n_2}...\,|0\rangle$$

where $n_1,n_2...$ run over $0,1,2,...$ such that there are only finite $j$ such that $n_j>0$. We have

$$\begin{aligned}
\mathrm{Tr}(G) &= \sum_{n_j=0,1,2,...} \langle n_1,n_2,...|\, G\, |n_1,n_2,...\rangle \\
&= \sum_{n_j=0,1,...;j\in I} (n_1!n_2!...)^{-1} \langle 0| \prod_{i\in I} (a_i^{n_i}\exp[-\lambda_i a_i^* a_i](a_i^*)^{n_i})\,|0\rangle \\
&= \sum_{n_j=0,1,...;j\in I} (n_1!n_2!...)^{-1} \langle 0| \prod_{i\in I} \left( a_i^{n_i} \sum_{k=0}^\infty \frac{(-\lambda_i)^k (a_i^* a_i)^k}{k!}(a_i^*)^{n_i}\right)|0\rangle \\
&= \sum_{n_j=0,1,...;j\in I} (n_1!n_2!...)^{-1} \langle 0| \prod_{i\in I} \left( \sum_{k=0}^\infty \frac{(-e_i)^k (n_i)^k (n_i!)}{k!}\right)|0\rangle \\
&= \sum_{n_j=0,1,...;j\in I} \prod_i e^{-\lambda_i n_i} = \prod_{i\in I} \frac{1}{1-e^{-\lambda_i}} < \infty
\end{aligned}$$

since $\sum_{i\in I} e^{-\lambda_i} < \infty$. Thus $\rho$ is well-defined.

We now prove that $\rho$ is a quasi-free state[18]. It suffices to prove (99)-(100) for $c_i := A_+(F_i)$ either a creation or annihilation operator. Our aim is to show that

$$\mathrm{Tr}[c_1c_2c_3c_4...c_kG] = \frac{\mathrm{Tr}[c_1c_2G]}{\mathrm{Tr}[G]}\mathrm{Tr}[c_3c_4...c_kG] \tag{101}$$

[18]The proof here is based on ideas of M. Gaudin, Une démonstartion simpliflée du théorème de Wick en méchanique statistique. *Nucl. Phys.* **15** (1960)

$$+\frac{\mathrm{Tr}[c_1c_3G]}{\mathrm{Tr}[G]}\mathrm{Tr}[c_2c_4...c_kG]+...+\frac{\mathrm{Tr}[c_1c_kG]}{\mathrm{Tr}[G]}\mathrm{Tr}[c_2c_3...c_{k-1}G]$$

and the result follows immediately by a simple induction. By the same way of computating $\mathrm{Tr}[G]$ we may check that

$$\frac{\mathrm{Tr}[c_1c_2G]}{\mathrm{Tr}[G]}=f(c_1)[c_1,c_2] \tag{102}$$

where $[c_1,c_2]=c_1c_2-c_2c_1\in\{0,-1,1\}$ and

$$f(c_1)=\begin{cases}(1-e^{-\lambda_j})^{-1} & \text{if } c_1=a_j,\ j\in I,\\ (1-e^{\lambda_j})^{-1} & \text{if } c_1=a_j^*,\ j\in I,\\ 1 & \text{if } c_1=a_j,\ j\notin I,\\ 0 & \text{if } c_1=a_j^*,\ j\notin I.\end{cases} \tag{103}$$

Thus (107) is equivalent to

$$\begin{aligned}\mathrm{Tr}[c_1c_2c_3c_4...c_kG]&=f(c_1)[c_1,c_2]\mathrm{Tr}[c_3c_4...c_kG]\\&+f(c_1)[c_1,c_3]\mathrm{Tr}[c_2c_4...c_kG]+...+f(c_1)[c_1,c_k]\mathrm{Tr}[c_2c_3...c_{k-1}G].\end{aligned} \tag{104}$$

We can prove (104) as follows. From the identity

$$c_1c_2c_3c_4...c_k=[c_1,c_2]c_3c_4...c_k+...+c_2c_4...c_{k-1}[c_1,c_k]+c_2c_3c_4...c_kc_1$$

we deduce that

$$\begin{aligned}\mathrm{Tr}\left[c_1c_2c_3c_4...c_kG\right]&=\mathrm{Tr}\left[[c_1,c_2]c_3c_4...c_kG\right]\\&\quad+...+\mathrm{Tr}\left[c_2c_4...c_{k-1}[c_1,c_k]G\right]+\mathrm{Tr}\left[c_2c_3c_4...c_kc_1G\right].\end{aligned} \tag{105}$$

We first consider when $c_1$ is either $a_j$ or $a_j^*$ with $j\in I$. In this case it is straightforward to see that $c_1G=e^{\pm\lambda_j}c_1G$ where (+) if $c_1=a_j^*$ and (-) if $c_1=a_j$. This implies that

$$\mathrm{Tr}\left[c_2c_3c_4...c_kc_1G\right]=e^{\pm\lambda_j}\mathrm{Tr}\left[c_2c_3c_4...c_kGc_1\right]=e^{\pm\lambda_j}\mathrm{Tr}\left[c_1c_2c_3c_4...c_kG\right]. \tag{106}$$

Substituting (106) into (106) we conclude that

$$\begin{aligned}\mathrm{Tr}\left[c_1c_2c_3c_4...c_kG\right]&=\frac{[c_1,c_2]}{1-e^{\pm\lambda_j}}\mathrm{Tr}\left[c_3c_4...c_kG\right]\\&+\frac{[c_1,c_3]}{1-e^{\pm\lambda_j}}\mathrm{Tr}\left[c_2c_4...c_kG\right]+...+\frac{[c_1,c_k]}{1-e^{\pm\lambda_j}}\mathrm{Tr}\left[c_2c_4...c_{k-1}G\right].\end{aligned}$$

which is precisely the desired identity (104).

If $c_1 = a_j$ for some $j \notin I$ then

$$\mathrm{Tr}[c_2c_3c_4...c_kc_1G] = 0$$

since $a_jG = 0$ and (104) follows (106).

Finally if $c_1 = a_j^*$ for some $j \notin I$ then

$$\mathrm{Tr}[c_1c_2c_3c_4...c_kG] = \mathrm{Tr}[c_2c_3c_4...c_kGc_1] = 0$$

since $Ga_j^* = 0$ and we obtain (104) again. □

**PROBLEM G.4.** *Prove that for fermions, using notations in Theorem G.3,*

$$\mathrm{Tr}(G) = \prod_{i\in\mathrm{I}} (1 + e^{-\lambda_i}) < \infty.$$

In the next theorem we characterize the 1-pdm of all quasi-free states. Moreover, we shall see in the proof that any quasi-free state is associated with a state described in Theorem G.3 via a Bogolubov transformation.

**THEOREM G.5** (1-pdm of quasi-free states)**.** *Let $\Gamma : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$ be an operator having the form as in (98). Then $\Gamma$ is the 1-pdm of a quasi-free state with finite particle number if and only if $\Gamma \geq 0$ and $\mathrm{Tr}[\gamma] < \infty$.*

*Proof.* The direct part is simple because if $\Gamma$ is the 1-pdm of a quasi-free state $\rho$ with finite particle expectation then it must be positive semi-definite since $\rho(A^*A) \geq 0$ for all operators $A$ and $\mathrm{Tr}[\gamma] = \rho[\mathcal{N}] < \infty$.

Now we prove the reverse part. Assume that $\Gamma \geq 0$ and $\mathrm{Tr}[\gamma] < \infty$. Note that from $\Gamma \geq 0$ we obtain that $\gamma \geq 0$ and $\alpha^* = \pm J\alpha J$. Using Theorem 9.9 we may write

$$\Gamma = \mathcal{V}^*\Gamma_0\mathcal{V} \text{ with } \Gamma_0 = \begin{pmatrix} \xi & 0 \\ 0 & 1 \pm J\xi J \end{pmatrix}$$

where $\mathcal{V} : \mathfrak{h}\oplus\mathfrak{h}^* \to \mathfrak{h}\oplus\mathfrak{h}^*$ is a Bogolubov map which is unitary implementable and $\xi$ is a positive semi-definite trace class operator on $\mathfrak{h}$ and $\xi \leq 1/2$ for fermionic case. (Infact, Theorem 9.9 is stated for 1-pdm of pure states but in the proof we just use the specific form of $\Gamma$.) Because the set of 1-pdm of quasi-free states is invariant under Bogolubov transformations we may consider $\Gamma_0$ instead of $\Gamma$.

We shall construct a quasi-free state whose 1-pdm is $\Gamma_0$. We shall first consider the bosonic case. Because $\xi$ is trace class it admits an orthogonal eigenbasis $\{u_i\}_{i=1}^{\infty}$ for $\mathfrak{h}$ corresponding to eigenvalues $\{\lambda_i\}_{i=1}^{\infty}$. Let $I = \{i \in \mathbb{N} | \lambda_i > 0\}$. Then we may choose $e_i \in (0, \infty)$ such that

$$(1 - \exp(-e_i))^{-1} = 1 + \lambda_i, \quad i \in I. \tag{107}$$

Let

$$G = \Pi_0 \exp\left[ -\sum_{i \in I} e_i a_+^*(u_i) a_+(u_i) \right]$$

where $\Pi_0$ is the projection onto the subspace $\mathrm{Ker}[\sum_{n \notin I} a_+^*(u_n) a_+(u_n)]$. Since

$$\sum_{i \in I} \exp(-e_i) = \sum_{i \in I} \frac{\lambda_i}{1 + \lambda_1} < \infty$$

it follows from Theorem G.3 that the state $\rho$ defined by

$$\rho[B] = \frac{\mathrm{Tr}[BG]}{\mathrm{Tr}[G]} \tag{108}$$

is a quasi-free state. Moreover from (102) we can see immediately that $\Gamma$ is precisely the 1-pdm of $\rho$.

The proof for fermionic case is totally the same where we just need to replace (107) by

$$(1 + \exp(-e_i))^{-1} = \lambda_i.$$

for $\lambda_i \in (0, 1)$. $\square$

One of the difficulties when dealing with the Hartree-Fock Theory and Bogolubov Theory is due to the nonlinearity of the set of variational states. For example, the convex combination of two quasi-free pure states is not necessarily a quasi-free pure state, and hence we cannot talk about extremal states.

Although the set of quantum quasi-free states is still nonlinear, using Theorem G.5 we can in some sense compensate for this by the linearity of the set of the corresponding one-particle density matrices.

**PROBLEM G.6** (Consistency of the quasi-free states and quasi-free pure states)**.** *Let $\rho$ be a quantum quasi-free state. Assume that $\rho$ is also a pure state in the Fock space $\mathcal{F}^{B,F}(\mathfrak{h})$. Prove that $\rho$ is a quasi-free pure state as in Definition 10.1.*

*(Hint: Under a Bogolubov transformation $\rho$ is defined uniquely by (108). Using the purity to prove that Ran$(G)$ is 1-dimensional.)*