Many-body quantum systems

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1 Introduction

We have already introduced many-body wave functions as a basic axiom of quantum mechanics. The quantum state of N particles with coordinates $x_1, \dots, x_N \in \mathbf{R}^d$ is described by a complex valued normalized wave function (without spins)

$$\psi(\mathbf{x}) = \psi(x_1, x_2, \dots, x_N) \in L^2(\mathbf{R}^{dN})$$

We will use the notation $\mathbf{x} = (x_1, x_2, \dots, x_N)$ for the collection of all the coordinates, and similarly we set $d\mathbf{x} = \mathrm{d}x_1 \mathrm{d}x_2 \dots \mathrm{d}x_N$ for the Lebesgue measure on $\mathbf{R}^{dN}$, thus

$$\int_{\mathbf{R}^{dN}} |\psi(\mathbf{x})|^2 \mathrm{d}\mathbf{x} = 1$$

The probability density

$$|\psi(x_1, x_2, \dots, x_N)|^2$$

is interpreted as simultaneously finding particle 1 at the location x_1, particle 2 at the location x_2 etc.

Similarly to probability theory, we can define the marginal distributions. The probability distribution of the i-th particle is given by

$$\varrho^i_\psi(x) = \int_{\mathbf{R}^{(d-1)N}} |\psi(x_1, \dots, x_{i-1}, x, x_{i+1} \dots)|^2 \mathrm{d}x_1 \dots \widehat{\mathrm{d}x_i} \dots \mathrm{d}x_N \tag{1.1}$$

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where hat means that the integration over x_i is omitted. Typically one is interested in the total electron density. We define the **one-particle density function** as

$$\varrho_\psi(x) = \sum_{i=1}^N \varrho_\psi^i(x) \tag{1.2}$$

Obviously

$$\int_{\mathbf{R}^d} \varrho_\psi(x)\mathrm{d}x = \sum_{i=1}^N \int_{\mathbf{R}^d} \varrho_\psi^i(x)\mathrm{d}x = \sum_{i=1}^N 1 = N$$

expressing the fact that the total number of particles in the system is N.

We also define the **density matrix** of a normalized $\psi \in L^2(\mathbf{R}^{dN})$ as

$$\Gamma_\psi = |\psi\rangle\langle\psi|$$

i.e. it is the orthogonal projection onto the one-dimensional space spanned by ψ. The operator kernel is given by

$$\Gamma_\psi(\mathbf{x}, \mathbf{x}') = \Gamma_\psi(x_1, x_2, \ldots, x_N; x_1', x_2', \ldots, x_N') := \psi(x_1, x_2, \ldots, x_N)\overline{\psi(x_1', x_2', \ldots, x_N')}$$

i.e. Γ_ψ acts on any element $\phi \in L^2(\mathbf{R}^{dN})$ as

$$(\Gamma_\psi\phi)(\mathbf{x}) = \int \psi(\mathbf{x})\overline{\psi(\mathbf{x}')}\phi(\mathbf{x}')\mathrm{d}\mathbf{x}' = \langle\psi, \phi\rangle\phi(\mathbf{x}).$$

We can define the **one particle density matrix** of Γ_ψ (the standard physics terminology is a bit misleading, it is not a matrix, but an operator) as

$$\gamma_\psi^{(1)}(x, x') \tag{1.3}$$

$$:= \sum_{i=1}^N \int_{\mathbf{R}^{d(N-1)}} \Gamma_\psi(x_1, x_2, \ldots, x_{i-1}, x, x_{i+1}, \ldots x_N; x_1, x_2, \ldots, x_{i-1}, x', x_{i+1}, \ldots x_N)\mathrm{d}x_1 \ldots \widehat{\mathrm{d}x_i} \ldots \mathrm{d}x_N$$

In other words, in the arguments of Γ_ψ we set all but $j = i$ variables equal, $x_j = x_j'$, and then integrate them out. In general **k-point density matrices** are defined analogously.

Note that $\gamma_\psi^{(1)}$ has two d-dimensional (i.e. "one-particle") arguments, so it can be viewed as an operator kernel acting in the one-particle space $L^2(\mathbf{R}^d)$. Moreover, its diagonal element is the one-particle density function, defined above:

$$\gamma_\psi^{(1)}(x, x) = \varrho_\psi(x).$$

All these definitions become much simpler if ψ is a symmetric or antisymmetric function:

Definition 1.1 *A function $\psi(z_1, z_2, \dots z_N)$ of N variables is called* **(totally) symmetric** *if*

$$\psi(\dots, z_i, \dots, z_j, \dots) = \psi(\dots, z_j, \dots, z_i, \dots)$$

for any index pairs (i, j) and it is called **(totally) antisymmetric** *if*

$$\psi(\dots, z_i, \dots, z_j, \dots) = -\psi(\dots, z_j, \dots, z_i, \dots)$$

for any index pairs (i, j). We will drop the word "totally".

In this case, the summations over i in (1.2) and (1.3) can be replaced with a simple factor N in front of the $i = 1$ term, e.g.

$$\varrho_\psi(x) = N \int_{\mathbf{R}^{(d-1)N}} |\psi(x, x_2, \dots, x_N)|^2 \mathrm{d}x_2 \dots \mathrm{d}x_N.$$

and similarly for $\gamma_\psi^{(1)}$.

2 Spin

Particles can have internal degrees of freedom; here we deal only with spins. The spin is typically a discrete label describing possible internal degrees of freedom that can characterize the state of the particle (in addition to the position coordinate). The number of internal states is a basic characteristics of the quantum particle that does not change with time; however, which of these states the particle occupies is dynamical. We use the label σ for the spin, and we assume that $\sigma \in \{1, 2, \dots q\}$, i.e. there are q spin states available. The standard physics labelling is

$$\sigma \in \left\{ -\frac{q-1}{2}, -\frac{q-3}{2}, \dots \frac{q-3}{2}, \frac{q-1}{2} \right\}$$

indicating the possible values of any fixed component of the spin vector (typically the z-component if spin represented as a vector in $\mathbf{R}^3$). Usually in physics a particle with q possible spin states is called a spin-$\frac{q-1}{2}$ particle, indicating the biggest physical spin label it can reach. Thus, for even q the spins are always half-integers, for odd q the spins are always integers.

Electrons, protons and neutrons have two spin states, $q = 2$, typically labelled by $1/2$ and $-1/2$ in physics, but here we use the labels $1, 2$.

In general, when we have N particles, each of them can have different number of spin states, say q_i for the i-th particle. The spin state is also part of the wave function description, so the correct wave function will have coordinate and spin variables:

$$\psi(x_1, \sigma_1, x_2, \sigma_2, \dots, x_N, \sigma_N)$$

where $x_i \in \mathbf{R}^d$ and $\sigma_i \in \{1, 2, \ldots, q_i\}$.

There are two ways to think about wave functions with spins. Either one keeps the spin variable together with the coordinate variable and defines

$$z_i = (x_i, \sigma_i) \in \mathbf{R}^d \times \{1, 2, \ldots q_i\}$$

as the composite coordinate. In this case we need to introduce the natural measure on the space

$$\mathbf{R}^d \times \{1, 2, \ldots q_i\}$$

which is of course just the usual Lebesgue integral in the position variable and the discrete sum for the spin, i.e.

$$\mathrm{d}z_i = \sum_{\sigma_i=1}^{q_i} \int_{\mathbf{R}^d} \mathrm{d}x_i$$

The one-particle Hilbert space is

$$L^2\big(\mathbf{R}^d \times \{1, 2, \ldots q_i\}\big) \equiv L^2(\mathbf{R}^d, \mathbf{C}^q)$$

under the natural identification

$$f(x, \sigma) \leftrightarrow \begin{pmatrix} f(x,1) \\ f(x,2) \\ \vdots \\ f(x,q) \end{pmatrix} \in \mathbf{C}^q$$

Writing $\underline{\sigma} = (\sigma_1, \ldots \sigma_N)$ and

$$\sum_{\underline{\sigma}} = \sum_{\sigma_1=1}^{q_1} \sum_{\sigma_2=1}^{q_2} \cdots \sum_{\sigma_N=1}^{q_N}$$

we can write the measure on the N-particle space

$$\prod_{i=1}^{N} \Big(\mathbf{R}^d \times \{1, 2, \ldots q_i\}\Big)$$

as

$$\mathrm{d}\mathbf{z} = \sum_{\underline{\sigma}} \int \mathrm{d}\mathbf{x}$$

The other way to think about wave functions with spin is that it is a collection of altogether $Q = \prod_{i=1}^{N} q_i$ "usual" wavefunctions, i.e.

$$\psi = \left\{ \psi_{\underline{\sigma}}(\mathbf{x}) \in L^2(\mathbf{R}^{dN}) \ : \ \underline{\sigma} \in \prod_{i=1}^{N} \{1, 2, \dots q_i\} \right\}$$

For example a wave function of two electrons (each with 2 possible spin states $q_1 = q_2 = 2$) is either

$$\psi(x_1, \sigma_1, x_2, \sigma_2) \qquad \sigma_1, \sigma_2 = 1, 2, \quad x_1, x_2 \in \mathbf{R}^d$$

or

$$\begin{pmatrix} \psi_{11}(x_1, x_2) \\ \psi_{12}(x_1, x_2) \\ \psi_{21}(x_1, x_2) \\ \psi_{22}(x_1, x_2) \end{pmatrix} \tag{2.4}$$

Of course in case of $q = 2$ the notation $\uparrow, \downarrow$ is used instead of $1, 2$, e.g. $\psi_{\uparrow\uparrow}(x_1, x_2)$.

The second notation is somewhat easier for analysis, but it somewhat disguises the fact that spin and position coordinates belong to each other; when particles are interchanged, they move together (see next section).

If each particle has the same number of spin states, $q_i = q$, then the one particle density function is defined analogously to the spinless case:

$$\varrho_\psi(x, \sigma) = \sum_{i=1}^{N} \varrho_\psi^i(x, \sigma)$$

$$\varrho_\psi^i(x, \sigma) = \sum_{\underline{\sigma}}^{*i} \int_{\mathbf{R}^{(d-1)N}} |\psi(x_1, \sigma_1 \dots, x_{i-1}, \sigma_{i-1}, x, \sigma, x_{i+1}, \sigma_{i+1} \dots)|^2 \mathrm{d}x_1 \dots \widehat{\mathrm{d}x_i} \dots \mathrm{d}x_N$$

where

$$\sum_{\underline{\sigma}}^{*i} = \sum_{\sigma_1}^{q} \cdots \sum_{\sigma_{i-1}}^{q} \sum_{\sigma_{i+1}}^{q} \cdots \sum_{\sigma_n}^{q}$$

i.e. we leave out the σ_i summation. If we are interested only in the one particle position space density, then we can sum over all σ's and consider

$$\varrho_\psi(x) = \sum_{\sigma=1}^{q} \varrho_\psi^i(x, \sigma)$$

3 Bosons and fermions

It is a postulate of quantum mechanics that quantum particles in $d \geq 3$ dimensions come in two types: bosons or fermions. This type is an inherent property of the particle and does not change with time. Moreover, their boson-fermion type is closely related to the spin-type. This is the **spin-statistics theorem**, which states that bosons have always integer spins (with our notation, q is odd), while fermions have always half-integer spins (q is even).

Electrons, protons and neutrons are always fermions, nuclei can be either fermions or bosons depending on their constituents. The sum rule for spins determines the type of a composite particle: e.g. a composite particle consisting of say four fermions (like the helium ion He^{++}, i.e. two protons and two neutrons) is a boson, while a particle with one boson and one fermion (like He^{+} consisting of a bosonic helium nucleus and an electron) is a fermion.

If we have a system consisting of several identical particles (e.g. many electrons), then there is no way to distinguish among them: the labels assigned to particle 1 and particle 2 have no meaning. Therefore, we expect that the wave function respects this fact and does not distinguish between $\psi(z_1, z_2)$ and $\psi(z_2, z_1)$ (or, more precisely, ψ is expected to depend on the two spin-position variables only as an *unordered set* $\{z_1, z_2\}$ and not as an *ordered sequence* (z_1, z_2)). This is almost correct, but not quite: for **bosons the wave function is indeed symmetric, for fermions it is antisymmetric.**

Remark. Note that the spin variable goes together with the position variable. For example, a wave function (2.4) of two identical spin-1/2 particles is antisymmetric if

$$\psi_{11}(x_1, x_2) = -\psi_{11}(x_2, x_1), \quad \psi_{22}(x_1, x_2) = -\psi_{22}(x_2, x_1)$$

and

$$\psi_{12}(x_1, x_2) = -\psi_{21}(x_2, x_1)$$

for any choice of $x_1, x_2 \in \mathbf{R}^d$. [And, by the spin-statistics theorem, we know that the wave-function (2.4) is actually a fermionic wave function if it describes identical particles].

Fundamental Postulate: Identical bosons are described by totally symmetric wave functions. Identical fermions are described by totally antisymmetric wave functions. This latter is often called the **Pauli principle**.

It is important to note that the symmetry requirement applies only to indistinguishable (identical) particles. For example, if the wave function (2.4) describes two spin-1/2 fermions that are not identical (e.g. are distinguished by some other internal degree of freedom, e.g. flavour), then no symmetry relation holds whatsoever: the four wave functions in $L^2(\mathbf{R}^{2d})$ in (2.4) are fully independent.

The wave function of a system consisting of several species of several indistinguishable particles must be subject to the partial symmetry requirements for each species. For example if

$$\psi(z_1, z_2, z_3, z_4, z_5)$$

is a wave function of two fermions and three bosons, say the fermions being the first two variables, the bosons being the rest, then ψ has to asymmetric in the first two variables

$$\psi(z_1, z_2, z_3, z_4, z_5) = -\psi(z_2, z_1, z_3, z_4, z_5)$$

and symmetric in the remaning three

$$\psi(z_1, z_2, z_3, z_4, z_5) = \psi(z_1, z_2, z_4, z_3, z_5) = \ldots = \psi(z_1, z_2, z_5, z_4, z_3)$$

No symmetry relation holds among the first group of two variables and the second group of three variables since they describe different particle species.

If $\psi(\mathbf{x})$ is a symmetric or antisymmetric wave function, then clearly $|\psi(\mathbf{x})|^2$ is a symmetric. In particular, the density function $\varrho^i(x)$ of the i-th particle defined in (1.1) is independent of i and the one particle density function is just N times of (any) ϱ^i.

The simplest form of a bosonic wavefunction is just the tensorproduct of any normalized one particle wavefunction $f(x) \in L^2(\mathbf{R}^d)$, $\|f\|_2 = 1$:

$$\psi(x_1, x_2, \ldots, x_N) = f(x_1)f(x_2)\ldots f(x_N)$$

Clearly $\|\psi\|_2 = 1$ and the one particle density is

$$\varrho_\psi(x) = N|f(x)|^2$$

More generally, one can consider a basis $f_1, f_2, \ldots \in L^2(\mathbf{R}^d)$ and consider functions of the form

$$(f_{j_1} \otimes f_{j_2} \otimes \ldots \otimes f_{j_N})(x_1, x_2, \ldots x_N) = \prod_{\ell=1}^{N} f_{j_\ell}(x_\ell), \qquad j_1, j_2, \ldots j_N \in \mathbf{N}$$

Such functions form a basis in the tensorproduct space $\bigotimes_1^N L^2(\mathbf{R}^d) = L^2(\mathbf{R}^{dN})$. Of course these functions are not bosonic, but one can symmetrize them by forming

$$f_{\otimes J}(\mathbf{x}) = \sum_{\pi \in S_N} \prod_{\ell=1}^{N} f_{j_\ell}(x_{\pi(\ell)}), \qquad J = \{j_1, j_2, \ldots, j_N\} \tag{3.5}$$

where S_N is the set of all permutations on N elements. In general, one can define the symmetrization operator

$$(\mathcal{S}\psi)(x_1, x_2, \ldots x_N) = \sum_{\pi \in S_N} \psi(x_{\pi(1)}, x_{\pi(2)}, \ldots)$$

It is easy to check that the operator $P_S = \frac{1}{N!}\mathcal{S}$ is an orthogonal projection, i.e. $P_S^* = P_S$ and $P_S^2 = P_S$. The image of P_S is the space of **symmetrized tensorproduct** (or bosonic tensorproduct). Standard notation for this space is $\bigotimes^s L^2(\mathbf{R}^d)$ or $\mathcal{S}(\bigotimes L^2(\mathbf{R}^d))$. If $f_1, f_2, \ldots$ form a basis in the one-particle Hilbert space $L^2(\mathbf{R}^d)$, then functions of the form (3.5) form a basis in the symmetrized tensorproduct, if the multiplicity is removed (i.e. the sets $J = \{j_1, j_2, \ldots j_N\}$, labelling the elements of (3.5), are indeed considered as sets and not sequences; clearly $j_1 = 3, j_2 = 5$ gives the same element as $j_1 = 5, j_2 = 3$).

The simplest form of an antisymmetric function is obtained by taking N functions in $L^2(\mathbf{R}^d)$ (neglecting spins for the moment), $f_1, f_2, \ldots f_N$ and forming their **antisymmetrized tensor product or Slater determinant**:

$$(f_1 \wedge f_2 \wedge \ldots \wedge f_N)(x_1, \ldots x_N) = \frac{1}{\sqrt{N!}} \det(f_i(x_j)) = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} (-1)^\pi \prod_{j=1}^N f_j(x_{\pi(j)})$$

where $(-1)^\pi$ denotes the parity of the permutation π. In most applications the functions $f_1, f_2, \ldots f_N$ will be orthonormal.

Notice the difference between the symmetrized and antisymmetrized tensor product (see (3.5)). The Slater determinant is just the **total antisymmetrization** $\mathcal{A}$ acting on the product state $\prod_j f_j(x_j)$:

$$(f_1 \wedge f_2 \wedge \ldots \wedge f_N)(x_1, \ldots x_N) = \frac{1}{\sqrt{N!}} \mathcal{A}\big[\prod_j f_j(x_j)\big]$$

where the action of $\mathcal{A}$ on any function of N variables is defined as

$$\big[\mathcal{A}\psi\big](x_1, \ldots x_N)\big] := \sum_{\pi \in S_N} (-1)^\pi \psi(x_{\pi(1)}, x_{\pi(2)}, \ldots, x_{\pi(N)})$$

From this definition it is easy to recognize the full expansion of the determinant in case when ψ is a product:

$$f_1 \wedge f_2 \wedge \ldots \wedge f_N = \frac{1}{\sqrt{N!}} \mathcal{A}\big[f_1 \otimes f_2 \otimes \ldots \otimes f_N\big]$$

(Note that some books use different normalization convention)

It can again be proven that Slater determinants form a basis in the space of antisymmetric functions (see Exercise below). This space is also called the **antisymmetric tensorproduct** and denoted by $\bigwedge_{i=1}^{N} L^2(\mathbf{R}^d)$. The same concepts extend if we consider spins; then x_i is to be replaced by the composite coordinate z_i and the one particle Hilbert space is $L^2(\mathbf{R}^d, \mathbf{C}^q)$.

For example, for $N = 2$ we have

$$(f_1 \wedge f_2)(x_1, x_2) = \frac{1}{\sqrt{2}}\big[f_1(x_1)f_2(x_2) - f_1(x_2)f_2(x_1)\big]$$

If spins are present, then different spin variables may lead to orthogonality, e.g. the functions

$$f_1(x, \sigma) = f(x)\delta(\sigma = 1), \qquad f_2(x, \sigma) = f(x)\delta(\sigma = 2)$$

are obviously orthogonal, since $\bar{f_1}(z)f_2(z) = 0$ pointwise. Thus the function

$$(f_1 \wedge f_2)(x_1, \sigma_1, x_2, \sigma_2) = f(x_1)f(x_2)\frac{1}{\sqrt{2}}\big[\delta(\sigma_1 = 1)\delta(\sigma_2 = 2) - \delta(\sigma_1 = 2)\delta(\sigma_2 = 1)\big] \qquad (3.6)$$

is an antisymmetric function despite the fact that in the position variable both f_1 and f_2 are the same.

Remark. For simplicity we worked with the underlying one particle Hilbert space being $\mathcal{H} = L^2(\mathbf{R}^d)$, but all these constructions naturally apply for any separable Hilbert space $\mathcal{H}$ as the one-particle space.

Exercise 3.1 *i) Prove that* $\|f_1 \wedge \ldots \wedge f_N\|_2 = 1$ *if* $f_1, f_2, \ldots f_N$ *are orthonormal.*

ii) Prove that

$$\langle f_1 \wedge \ldots \wedge f_N, g_1 \wedge \ldots \wedge g_N \rangle = det\{\langle f_i, g_j \rangle\}$$

where on the right hand side we take the determinant of the $N \times N$ *matrix with* (i, j)*-th entry being* $\langle f_i, g_j \rangle$*. [The scalar product on the left hand side is with respect to* $L^2(\mathbf{R}^{dN})$*, on the right hand side is wrt* $L^2(\mathbf{R}^d)$*.]*

iii) Let $f_1, \ldots f_N$ *be arbitrary elements of* $L^2(\mathbf{R}^d)$ *and let* A *be an* $N \times N$ *matrix. Define the functions*

$$g_i = \sum_{j=1}^{N} A_{ij} f_j, \qquad i = 1, 2, \ldots N$$

Prove that

$$g_1 \wedge \ldots \wedge g_N = (detA) f_1 \wedge \ldots \wedge f_N$$

In particular, choosing U *unitary, the wedge product is invariant under unitary transformations within the subspace* $Span(f_1, f_2, \ldots f_N)$*, modulo, possible a constant phase factor.*

iv) Prove that $f_1 \wedge f_2 \wedge \ldots \wedge f_N = 0$ if and only if $f_1, \ldots f_N$ are linearly dependent.
v) Prove that the one particle density of $\psi = f_1 \wedge \ldots \wedge f_N$ is given by

$$\varrho_\psi(x) = \sum_{i=1}^{N} |f_i(x)|^2$$

vi) Let $f = f_0, f_1, f_2, \ldots$ be an orthonormal basis in the Hilbert space $L^2(\mathbf{R}^d)$. Prove that the functions of the form

$$f_{\wedge J} = f_{j_1} \wedge f_{j_2} \wedge \ldots \wedge f_{j_N}$$

for $J = (j_1, j_2, \ldots, j_N) \in \mathbf{N}^N$ with distrinct elements ($j_\ell \neq j_k$ for $j \neq k$) form an orthonormal basis in $\bigwedge_1^N L^2(\mathbf{R}^d)$.

We make one more observation. Suppose that the Hamiltonian H is independent of the spin variable, i.e. it naturally acts on the space of spinless wave functions. Of course such an operator can be trivially extended to the wavefunctions with spin: it just acts trivially (as the identity operator) in the spin variables; more formally, H is the operator acting on $L^2(\mathbf{R}^{dN})$ and $H \otimes I$ acts on $L^2(\mathbf{R}^{dN}) \otimes \mathbf{C}^Q$.

Furthermore, we assume that H is symmetric under all permutations of the variables. This means that if σ_{ij} denotes the operator of exchanging i-th and j-th variables in the wave-function,

$$\big[\sigma_{ij}\psi\big](x_1, \ldots x_i, \ldots x_j, \ldots x_N) = \psi(x_1, \ldots x_j, \ldots x_i, \ldots x_N)$$

then H commutes with σ_{ij} for any pair i, j:

$$H\sigma_{ij} = \sigma_{ij}H$$

Now suppose that $q \geq N$, i.e. the number of spin is bigger than the number of particles. Then the fermionic character can be completely forgotten. More precisely, if $\phi(x_1, \ldots x_N)$ is an arbitrary function depending only on the space variables, then we can trivially extend this function to be a spin-dependent *antisymmetric* function as

$$\psi(z_1, \ldots z_N) = \frac{1}{\sqrt{N!}}\, \mathcal{A}\Big[\phi(x_1, \ldots x_N) \prod_{j=1}^{N} \delta(\sigma_j = j)\Big]$$

(the same trick with the special case $N = 2$ and $\phi(x_1, x_2) = f(x_1)f(x_2)$ was presented in (3.6))

Exercise 3.2 *Prove that*

i) $\|\phi\| = \|\psi\|$

ii) If H *is independent of the spin and is invariant under all the permutations, then* $\langle \phi, H\phi \rangle = \langle \psi, (H \otimes I)\psi \rangle$

This result means that as far as the ground state energy is concerned, the fermionic ground state energy with $q \geq N$ spins is the same as the unrestricted ground state energy without spin:

$$\inf \Big\{ \mathcal{E}(\phi) \ : \ \phi \in L^2(\mathbf{R}^{dN}), \|\phi\| = 1 \Big\} = \inf \Big\{ \mathcal{E}(\psi) \ : \ \psi \in \bigwedge_{j=1}^{N} L^2(\mathbf{R}^d; \mathbf{C}^q), \|\psi\| = 1 \Big\}$$

The advantage of this observation is that if we get a result on the ground state energy of the fermionic systems with arbitrary number of spins (of course this energy will depend on q), then we also get a result for the unrestricted problem, and later we will see (Theorem 4.1) that the minimizer of the unrestricted problem (under general conditions) is actually bosonic. Thus we will get a result on the bosonic ground state for free from the fermionic result.

4 Energy of the many-body system

We consider N interacting particles, each subject to the same external real potential V and any two particles interact via the real two-body translation invariant potential given by

$$W(x_1, \ldots, x_N) = \sum_{i<j} U(x_i - x_j)$$

We assume that U is symmetric, $U(x) = U(-x)$. The Hamilton operator H is the sum of a non-interacting Hamiltonian H_0 plus the interaction potential:

$$H = H_0 + W$$

where the non-interacting part is given by

$$H_0 = \sum_{i=1}^{N} \Big(-\Delta_{x_i} + V(x_i) \Big)$$

i.e. it is just the usual one particle operator $h = -\Delta_x + V(x)$ acting on each particle separately.

More formally one can write the non-interacting part as

$$H_0 = h \otimes I \otimes \ldots \otimes I + I \otimes h \otimes I \otimes \ldots \otimes I + \ldots + I \otimes \ldots \otimes I \otimes h$$

indicating that h is extended from the one particle space to the N particle space acting on the first, second etc. variables separately. We will not use this long and clumsy notation, we will just write as

$$H_0 = \sum_{i=1}^{N} h_i$$

where the index i in h_i indicates that the one-particle operator h acts on the i-th variable. Similarly one can formalize the extension of the interaction to the N-body space, originally considered as a multiplication on a two particle space.

Recall the corresponding energy functional of an N-body wavefunction $\psi(\mathbf{x})$ without interaction:

$$\mathcal{E}_0(\psi) = \sum_{i=1}^{N} \int \Big[|\nabla_i \psi(\mathbf{x})|^2 + V(x_i)|\psi(\mathbf{x})|^2 \Big] \mathrm{d}\mathbf{x} \tag{4.7}$$

and with interaction

$$\mathcal{E}(\psi) = \mathcal{E}_0(\psi) + \sum_{i<j} \int U(x_i - x_j)|\psi(\mathbf{x})|^2 \mathrm{d}x \tag{4.8}$$

Recall that we have defined the ground state energy

$$E_0 = \inf \big\{ \mathcal{E}(\psi) \ : \ \psi \in H^1(\mathbf{R}^{dN}), \ \ \|\psi\| = 1 \big\}$$

We can define the bosonic or fermionic ground state energies, by taking the infimum over all bosonic or fermionic wavefunctions, respectively:

$$E_0^b = E_0^b(N) = \inf \big\{ \mathcal{E}(\psi) \ : \ \psi \in H^1(\mathbf{R}^{dN}), \ \ \psi \in \mathcal{S} \bigotimes_1^N L^2(\mathbf{R}^d), \ \ \|\psi\| = 1 \big\}$$

$$E_0^f = E_0^f(N) = \inf \big\{ \mathcal{E}(\psi) \ : \ \psi \in H^1(\mathbf{R}^{dN}), \ \ \psi \in \bigwedge_1^N L^2(\mathbf{R}^d), \ \ \|\psi\| = 1 \big\} \tag{4.9}$$

We note that the Hamiltonian is independent of the spin, thus the energy should not depend on the spin variable. This is true as long as we work with bosons (however the non-degeneracy of the ground state is effected by the presence of the spin variable), but not true for fermions: presence of spins helps to reduce the effect of the Pauli principle as we have seen in the example (3.6).

We first show that the unrestricted ground state is bosonic:

Theorem 4.1 *Suppose that the energy functional $\mathcal{E}(\psi)$ defined in* (4.8) *is bounded from below, i.e. $E_0 > -\infty$. Then $E_0 = E_0^b$.*

Remarks: i) This theorem does not hold in general if magnetic fields are present.

ii) It is not necessary that we have a two body potential, the theorem holds for any real potential function $W(x_1, \dots x_N)$ that is symmetric with respect to all permutations.

The proof relies on the following abstract lemma

Lemma 4.2 *Let $\mathcal{E}(\psi)$ be a quadratic form on $L^2(\mathbf{R}^{dN})$ that is bounded from below, $\mathcal{E}(\psi) \geq c\|\psi\|^2$ for some finite constant. Assume that $\mathcal{E}(|\psi|) \leq \mathcal{E}(\psi)$ and that $\mathcal{E}(\psi)$ is invariant under any permutation of the variables, i.e. $\mathcal{E}(\psi_\pi) = \mathcal{E}(\psi)$ for any $\pi \in S_N$, where $\psi_\pi(x_1, \dots, x_N) = \psi(x_{\pi(1)}, \dots, x_{\pi(N)})$. Then*

$$\inf\{\mathcal{E}(\psi) \ : \ \|\psi\| = 1\} = \inf\{\mathcal{E}(\psi) \ : \ \|\psi\| = 1, \psi_\pi = \psi \ \forall \pi \in S_N\} \tag{4.10}$$

Proof of the Lemma. It is sufficient to show the inequality $\geq$ in (4.10), the other direction is trivial. Since the L^2-norm is unchanged and the energy does not increase if we change ψ to $|\psi|$, we can assume that ψ is non-negative. The same assumption can be made when we minimize for symmetric functions, since if ψ is symmetric so is $|\psi|$. Now we write $\psi = \psi_s + \psi_r$, where $\psi_s = \frac{1}{N!}\sum_{\pi \in S_N} \psi_\pi$ is the symmetrization of ψ and $\psi_r := \psi - \psi_s$. Since $\mathcal{E}(\psi_\pi) = \mathcal{E}(\psi)$, we can compute that

$$\mathcal{E}(\psi) = \mathcal{E}(\psi_s) + \mathcal{E}(\psi_r) \tag{4.11}$$

and

$$(\psi, \psi) = (\psi_s, \psi_s) + (\psi_r, \psi_r) \tag{4.12}$$

To see this, we demonstrate in the case of the norm why the cross terms (ψ_s, ψ_r) vanish:

$$(\psi_s, \psi_r) = \frac{1}{(N!)^2}\sum_{\pi,\sigma}(\psi_\pi, \psi - \psi_\sigma) = \frac{1}{(N!)^2}\sum_{\pi,\sigma \in S_N}(\psi, \psi_{\pi^{-1}} - \psi_{\pi^{-1}\sigma}) = 0$$

because $\sum_\pi \psi_{\pi^{-1}} = \sum_\pi \psi_{\pi^{-1}\sigma} = N!\psi_s$. Similar proof holds for the energy, one has to define the appropriate sesquilinear form associated with $\mathcal{E}$:

$$\widetilde{\mathcal{E}}(\psi, \phi) = \sum_{i=1}^N \int \nabla_i \bar{\psi} \cdot \nabla_i \phi + \int V\bar{\psi}\phi + \sum_{i<j}\int W(x_i - x_j)\bar{\psi}\phi$$

and repeat the above argument.

Armed with (4.11) and (4.12) and with the fact that $\psi_s \neq 0$ (since $(\psi_s, \psi_s) \geq \frac{1}{N!}$ because $(\psi_\pi, \psi_{\pi'}) \geq 0$ by the non-negativity of ψ), we obtain that if ψ is a minimizer for E_0, then so is $\psi_s/\|\psi_s\|$. To see this, we have

$$\mathcal{E}(\psi_s) \geq E_0\langle\psi_s, \psi_s\rangle, \qquad \mathcal{E}(\psi_r) \geq E_0\langle\psi_r, \psi_r\rangle$$

so equality must hold in both inequalities if their sum, $\mathcal{E}(\psi) = E_0(\psi, \psi)$ has an equality. In particular, $\mathcal{E}(\psi_s) = E_0\langle\psi_s, \psi_s\rangle$ which proves the $\geq$ in (4.10).

Note that this argument tacitly assumed that the minimizer ψ on the left hand side of (4.10) exists. If it does not exist, one can still repeat the argument with a minimizing sequence [THINK IT OVER] $\square$.

Proof of the Theorem. The quadratic form (4.8) is clearly invariant under any permutation, $\mathcal{E}(\psi_\pi) = \mathcal{E}(\psi)$. To check that $\mathcal{E}(|\psi|) \leq \mathcal{E}(\psi)$, we first note that the potential energy part depends only on $|\psi|$. For the kinetic energy part we need to show that

$$\int |\nabla_i|\psi||^2 \mathrm{d}\mathbf{x} \leq \int |\nabla_i\psi|^2 \mathrm{d}\mathbf{x}$$

but this property was already proven in the one particle setup. $\square$.

5 Ground state of non-interacting bosons

Consider the energy functional $\mathcal{E}_0(\psi)$ of N non-interacting particles (without symmetry restriction) defined in (4.7). Let

$$E_0 = \inf\{\mathcal{E}_0(\psi) \ : \ \psi \in H^1(\mathbf{R}^{dN}), \ \ \|\psi\| = 1, \}$$

be the ground state energy.

Theorem 5.1 *Suppose that the ground state energy e_0 of $h = -\Delta + V$ is not minus infinity,*

$$e_0 = \inf\Big\{ \int |\nabla f|^2 + V|f|^2 \ : \ f \in H^1(\mathbf{R}^d), \ \|\psi\|_2 = 1\Big\} > -\infty \tag{5.13}$$

Then the ground state energy of N non-interacting particles is $E_0 = Ne_0$, in particular the system satisfies the stability of second kind and $E_0 = E_0^b$ by Theorem 4.1.

If, additionally, the ground state f_0 of the energy functional (5.13) *exists, then the ground state of $\mathcal{E}_0(\psi)$ also exists and it is just $\psi_0(\mathbf{x}) = \prod_{i=1}^N f_0(x_i)$ (in particular, it is unique). If the particles have q spin degrees of freedom, then the ground state of the energy functional* (5.13) *is q-fold degenerate and the ground state of $\mathcal{E}_0(\psi)$ is q^N-fold degenerate.*

Remark: This statement holds in general for any operator of the form $\sum_i h_i$, where h is an arbitrary operator on the one-particle space $\mathcal{H}$, whose quadratic form is bounded from below, but the proof for the general case requires the spectral theorem. The proof presented below avoids this.

However, it is instructive to remark that if h has a fully discrete spectrum, with eigenvalues $e_0 \leq e_1 \leq \ldots$ and orthonormal eigenvectors $v_0, v_1, \ldots$, then one easily prove that

$$\inf \Big\{ \langle \psi, \sum_{i=1}^{N} h_i \psi \rangle, \psi \in \mathcal{H}^{\otimes N} \Big\} = N e_0$$

To see this, note that the tensor-product space $\mathcal{H}^{\otimes N}$ has a natural orthonormal basis of the form

$$\{ \mathbf{v}_{\otimes J} \ : \ J \in \mathbf{N}^N \}$$

where for any $J = (j_1, j_2, \ldots, j_N) \in \mathbf{N}^N$ we define

$$\mathbf{v}_{\otimes J} = v_{j_1} \otimes v_{j_2} \otimes \ldots \otimes v_{j_N}$$

It is easy to see that

$$\Big(\sum_{i=1}^{N} h_i \Big) \mathbf{v}_{\otimes J} = \big(\sum_{i=1}^{N} e_{j_i} \Big) \mathbf{v}_{\otimes J}$$

thus the set $\{ \mathbf{v}_{\otimes J} \ : \ J \in \mathbf{N}^N \}$ forms a complete eigenbasis for $\sum_i h_i$. The lowest eigenvalue is of course

$$\min_J \sum_{i=1}^{N} e_{j_i} = N e_0$$

Proof of Theorem 5.1. Using the product trial function $\psi_0(\mathbf{x}) = \prod_{i=1}^{n} f_0(x_i)$, we easily see that $\|\psi_0\| = 1$ and

$$\mathcal{E}_0(\psi_0) = \sum_{i=1}^{N} \int \Big[|\nabla f_0(x_i)|^2 + V(x_i) |f_0(x_i)|^2 \Big] \mathrm{d}x_i = N e_0$$

thus

$$N e_0 \geq E_0$$

For the other direction, we can use that $E_0 = E_0^b$ (from Theorem 4.1), i.e. it is sufficient to show that $N e_0 \leq E_0^b$.

Let $\psi(\mathbf{x})$ be a normalized symmetric (bosonic) function, and let

$$\varrho(x) = N \int |\psi(x, x_2, \dots, x_N)|^2 \mathrm{d}x_2 \dots \mathrm{d}x_N$$

be its one particle density. Compute

$$|\nabla \sqrt{\varrho(x)}|^2 = \frac{|\nabla \varrho(x)|^2}{4\varrho(x)} = \frac{N^2}{4\varrho(x)} \left| \int \Big[\nabla_x \bar{\psi}(x, x_2, \dots) \cdot \psi(x, x_2, \dots) + c.c \Big] \mathrm{d}x_2 \dots \mathrm{d}x_N \right|^2$$

where $c.c$ denotes the complex conjugate of the previous term; in this case $\nabla_x \psi(x, x_2, \dots) \cdot \bar{\psi}(x, x_2, \dots)$. By two Schwarz inequalities,

$$\begin{aligned} |\nabla \sqrt{\varrho(x)}|^2 \leq & \frac{N^2}{\varrho(x)} \left| \int |\nabla_x \psi(x, x_2, \dots)| \, |\psi(x, x_2, \dots)| \mathrm{d}x_2 \dots \mathrm{d}x_N \right|^2 \\ \leq & \frac{N^2}{\varrho(x)} \left[\int |\psi(x, x_2, \dots)|^2 \mathrm{d}x_2 \dots \mathrm{d}x_N \right] \left[\int |\nabla_x \psi(x, x_2, \dots)|^2 \mathrm{d}x_2 \dots \mathrm{d}x_N \right] \\ \leq & N \int |\nabla_x \psi(x, x_2, \dots)|^2 \mathrm{d}x_2 \dots \mathrm{d}x_N \end{aligned} \tag{5.14}$$

[**Remark in bracket:** You may slightly worry that this calculation is not quite correct if $\varrho(x) = 0$. The short answer is a rule of thumb: if the final estimate is finite (which is our case), then one can always use regularization to avoid the zero set. The longer answer: compute $|\nabla \sqrt{\varrho(x) + \varepsilon}|^2$ and remove the ε at the end; of course this tells you how to define $\nabla \sqrt{\varrho(x)}$ when $\varrho(x) = 0$ – just define it as a (monotone) limit of this regularization. – THINK IT OVER!]

In particular, we proved that

$$\int |\nabla \sqrt{\varrho(x)}|^2 \mathrm{d}x \leq T_\psi$$

where, we recall, T_ψ is the kinetic energy

$$T_\psi = \sum_{i=1}^{N} \int |\nabla_i \psi(\mathbf{x})|^2 \mathrm{d}\mathbf{x}$$

and we used the symmetry of ψ. This also shows that $\sqrt{\varrho} \in H^1(\mathbf{R}^d)$.

For the potential energy, clearly

$$\sum_{i=1}^{N} \int V(x_i)|\psi(\mathbf{x})|^2 = \int V(x)\varrho(x)\mathrm{d}x$$

(by the way, this holds for both bosonic and fermionic wave functions, since $|\psi(\mathbf{x})|$ is symmetric in both cases). Thus we proved that

$$\mathcal{E}_0(\psi) \geq \int \left[|\nabla\sqrt{\varrho}|^2 + V\varrho\right]$$

and we know that $\int \varrho = N$. Defining $f(x) = N^{-1/2}\sqrt{\varrho}$, we see that

$$\mathcal{E}_0(\psi) \geq N \int \left[|\nabla f|^2 + V|f|^2\right]$$

and $\int |f|^2 = 1$, $f \in H^1$, i.e. f is an admissible function for the variational problem (5.13). Thus

$$\mathcal{E}_0(\psi) \geq Ne_0$$

and since this holds for any bosonic ψ, we have $E_0 \geq Ne_0$ after taking the infimum for all ψ's.

If the minimizer of (5.13) exists, then clearly $\psi(\mathbf{x}) = \prod_i f_0(x_i)$ is a minimizer for the N-body energy. Now we prove that this is the only minimizer.

If ψ is a minimizer, then its real an imaginary parts, $R = \operatorname{Re}\psi$, $I = \operatorname{Im}\psi$ are also minimizers, since [CHECK!]

$$\mathcal{E}_0(\psi) = \mathcal{E}_0(R) + \mathcal{E}_0(I) \ , \ \|\psi\|^2 = \|R\|_2^2 + \|I\|_2^2$$

and thus

$$E_0 = \mathcal{E}_0(\psi) = \mathcal{E}_0(R) + \mathcal{E}_0(I) \geq E_0\|R\|_2^2 + E_0\|I\|_2^2 = E_0$$

so we have equality everywhere.

So we can assume that ψ is real. Since it is a minimizer, then there is equality in all Schwarz inequalities in the proof above, in particular

$$\lambda(x)\psi(x, x_2, \ldots x_N) = \nabla_x\psi(x, x_2, \ldots x_N)$$

for almost all $x_2, \ldots x_N$. By symmetry, $\log\psi(\mathbf{x})$ is thus a function whose all mixed derivatives vanish, so $\log\psi(\mathbf{x}) = \sum_i g_i(x_i)$ for some functions g_i, but by symmetry again $g_1 = g_2 = \ldots = g_N$, i.e. $\psi(\mathbf{x}) = \prod_i \phi(x_i)$ with some ϕ. Computing the energy of this function, we have

$$Ne_0 = \mathcal{E}(\psi) = N \int \left[|\nabla\phi|^2 + V|\phi|^2\right]$$

thus g is the minimizer of the one-particle variational problem (5.13), but we have proved that the minimizer of (5.13) is unique, thus $\phi = f_0$.

If the particle has q degrees of spin freedom, then the ground state of the variational problem (5.13) is obviously q-fold degenerate, one can use the functions $f_j(z) = f_0(x)\delta(\sigma = j)$ that are linearly independent and all give the same energy e_0. It is easy to check that the space of all their linear combinations are ground state functions as well. Clearly no other function is a one particle ground state: for any function $f(x, \sigma)$ we can just forget about the σ index as it does not appear in the Hamiltonian. Thus we see that any ground state $f(x, \sigma)$ of (5.13) must be of the form $f(x, \sigma) = f_0(x)g(\sigma)$ and the space of functions of the form $g(\sigma)$ is just $\mathbf{C}^q$. The degeneracy of the ground state of the N-body problem is q^N, since in the product $\prod_{i=1}^N f_0(x, \sigma_i)$ we can choose the spin indices σ_i arbitrarily. □

6 Crash course on operators in a Hilbert space

The material of this section is standard stuff in functional analysis. I just list a few key facts, if you are unfamiliar with them, check them out in Reed-Simon (for example).

- Concept of a linear operator on a separable Hilbert space $\mathcal{H}$.
- Bounded linear operators, operator norm
- Densely defined bounded operators have a unique bounded extension to the whole $\mathcal{H}$; thus bounded operators can be assumed to be defined everywhere
- Adjoint of a bounded operator. $\|A\| = \|A^*\|$, $\|AA^*\| = \|A\|^2$, $(AB)^* = B^*A^*$, $(A^*)^* = A$.
- Orthogonal projection ($P^2 = P$, $P^* = P$)
- Self-adjoint bounded operators and unitary operators
- A bounded operator is self-adjoint if and only if its quadratic form, $Q(x) = (x, Ax)$, $x \in \mathcal{H}$, is real valued.
- Resolvent set of A: $\varrho(A) = \{z \in \mathbf{C} \ : \ (z - A)^{-1}$ exists and is bounded$\}$
- Spectrum of A: $\sigma(A) = \mathbf{C} \setminus \varrho(A)$. $\sigma(A^*) = \overline{\sigma(A)}$.

- The resolvent set is open (in $\mathbf{C}$) the spectrum is closed. The resolvent function

$$R(z) : z \to (z - A)^{-1}$$

is analytic from $\varrho(A)$ to the set of bounded linear operators on $\mathcal{H}$. [This is a nontrivial theorem]

- The spectrum is never empty. [This follows from Liouville theorem applied for operator valued analytic functions.]

- The spectrum is always contained in the ball of radius $\|A\|$ about the origin in $\mathbf{C}$.

- Let $R := \lim_{n\to\infty} \|A^n\|^{1/n}$ (limit exists), then

$$R = \sup_{\lambda\in\sigma(A)} |\lambda|$$

and is also called the **spectral radius**. Typically $R \leq \|A\|$ but for bounded self-adjoint operators $R = \|A\|$.

- Eigenvalue and eigenvector. The set of eigenvalues is called the point spectrum.

- The spectrum may contain other elements than eigenvalues (unlike in finite dimensions!). It may happen that there are no eigenvalues at all.

- If $A = A^*$ and $\lambda \in \sigma(A)$, then either λ is an eigenvalue, or $\mathrm{Ran}(\lambda - A)$ is dense (these λ's form the **continuous spectrum** of A). [This is a non-trivial theorem using the inverse mapping theorem]

- If $A = A^*$, then $\sigma(A) \subset \mathbf{R}$ and eigenvectors belonging to different eigenvalues are orthogonal.

- Hellinger-Toeplitz theorem: If A is symmetric and defined on the whole H-space, then it is bounded thus self-adjoint.

- Compact operators: These are bounded operators A that map bounded sets into pre-compact sets. In other words, if $x_1, x_2, \ldots$ is a bounded sequence, $\sup_n \|x_n\| < \infty$, then the sequence $Ax_1, Ax_2, \ldots$ have a convergent subsequence.

- Compact operators can be arbitrarily approximated (in operator norm) by finite rank operators, i.e. by operators whose range has finite dimension. In other words: the set of compact operators is the norm closure of the finite rank operators. Most theorems that are known in finite dimensions extend fairly naturally to compact operators.

- In finite dimensional spaces compact operators are the same as bounded operators. In infinite dimensions, being a compact operator is a serious restriction, for example the identity operator is not compact. However, many integral operators of the form

$$(Kf)(x) = \int k(x,y)f(y)\mathrm{d}y$$

(defined on some function spaces, e.g $L^2(\mathbf{R}^d)$ or $C(\mathbf{R}^d)$) are compact under suitable conditions on the kernel function.

- Compact operators form an ideal within all bounded operators i.e. the operator product (composition) of a bounded operator and a compact operator is compact.

- Fredholm alternative: A compact, $\lambda \in \mathbf{C} \setminus \{0\}$. Then

$$\mathrm{dim}N(\lambda - A) = \mathrm{codim}R(\lambda - A)$$

and both are finite, moreover $R(\lambda - A)$ is closed (here N is the nullspace, R is the range). [The proof is non-trivial.] In other words, the only obstruction to the bounded invertibility of $\lambda - A$ is if λ is an eigenvalue; if $N(\lambda - A) = \{0\}$, i.e. λ is not an eigenvalue, then $R(\lambda - A) = \mathcal{H}$, moreover $(\lambda - A)^{-1}$ is bounded [Inverse mapping theorem].

- The spectrum of a compact operator away from zero consists of eigenvalues of finite multiplicity that may accumulate only at zero.

- **Spectral theorem for self-adjoint compact operators.** [Proof is nontrivial] Let $A = A^*$ be compact, then there is a sequence of non-zero real numbers, $\lambda_1, \lambda_2, \ldots$ (eigenvalues) with finite multiplicity and an orthonormal set of vectors $v_1, v_2, \ldots \in \mathcal{H}$ (eigenvectors) such that

$$Ax = \sum_j \lambda_j \langle v_j, x\rangle v_j \qquad \forall x \in \mathcal{H} \tag{6.15}$$

or, with short physics notation

$$A = \sum_j \lambda_j |v_j\rangle\langle v_j|$$

The sum in (6.15) may be finite (finite range operator) or infinite. In the latter case the sum of course converges in $\mathcal{H}$. The set of eigenvalues, together with their multiplicities is uniquely determined from A. The eigenvectors are subject to the same ambiguity as

by diagonalization of matrices: it is only the eigenspace belonging to a fixed eigenvalue that is uniquely determined; within the eigenspace there is a freedom to choose an orthonormal basis. For simple eigenvalues (meaning multiplicity one) this amounts only to a possible phase factor difference, for multiple eigenvalues with multiplicity m the freedom is given by an $m \times m$ unitary matrix.

[One can formulate the theorem in such a way that we allow zero eigenvalues – with possible infinite multiplicity – and then we can assume that the eigenvectors form an orthonormal basis.]

- **Singular value decomposition for compact operators.** If A is compact, then there exists a sequence of non-negative numbers $\mu_1, \mu_2, \ldots$, with finite multiplicity (called singular values) and there exists two sets of orthonormal vectors $\{u_j\}$ and $\{v_j\}$ (called left and right singular vectors) such that

$$Ax = \sum_j \mu_j \langle u_j, x \rangle v_j \qquad \forall x \in \mathcal{H}$$

The sum may be finite (finite range operator) or infinite. We can also write it as

$$A = \sum_j \mu_j |v_j\rangle\langle u_j|.$$

[One can formulate the theorem in such a way that we allow zero singular values – with possible infinite multiplicity – and then we can assume that both sets of singular vectors form an orthonormal basis.]

The singular value decomposition is a generalization of the spectral theorem: notice that in the self-adjoint case one can choose the left and right singular vectors to be the same (and the singular values are real).

- The norm of a compact operator is its largest singular value (in absolute value):

$$\|A\| = \max_j \mu_j$$

For the self-adjoint case of course we have $\|A\| = \max_j |\lambda_j|$.

- A selfadjoint bounded operator is called **positive** its quadratic form is non-negative, $\langle x, Ax \rangle \geq 0$. (It would be more correct to call it positive semidefinite, like for matrices, but it is often called positive only.) For compact operators, positivity is equivalent to $\lambda_j \geq 0$ for all eigenvalues. For two self-adjoint operators we say that $A \leq B$ if $B - A \geq 0$.

- Any positive operator has a unique positive **square root**, i.e. there is an unique operator $B \geq 0$ such that $B^2 = A$. If A is compact with spectral decomposition $A = \sum_j \lambda_j |v_j\rangle\langle v_j|$, then $B = \sum_j \sqrt{\lambda_j} |v_j\rangle\langle v_j|$.

- For any bounded operator A we can define its absolute value as

$$|A| = \sqrt{A^* A}$$

  WARNING: The notation indicates that A behaves as the usual absolute value for numbers, but this is wrong in most cases. The "expected" identity that is correct is $|\lambda A| = |\lambda|\,|A|$, but in general it is *false* that $|AB| = |A|\,|B|$, $|A| = |A^*|$ or that $|A + B| \leq |A| + |B|$.

- If A is compact, then the singular values of A and the eigenvalues of $|A|$ coincide.

- **Polar decomposition.** For any bounded operator A there is a partial isometry U such that $A = U|A|$ and U is unique under the condition that $\operatorname{Ker} U = \operatorname{Ker} A$. This is the matrix analogue of the decomposition of any complex number z into its absolute value and phase, $z = |z|e^{i\theta}$, but U may not be unitary. [U being partial isometry means that U is an isometry on $(\operatorname{Ker} U)^\perp$, i.e. it can have non-trivial kernel.

- Let A be a bounded operator on $\mathcal{H}$. If for *some* orthonormal basis (ONB) $\{x_j\}$ we have

$$\sum_j |\langle x_j, Ax_j\rangle| < \infty \tag{6.16}$$

  then we define the **trace** of A as

$$\operatorname{Tr} A := \sum_j \langle x_j, Ax_j\rangle \tag{6.17}$$

  It turns out that if (6.16) holds for some ONB, then it holds for all ONB. Moreover, the trace is independent of the choice of ONB. [These last two facts are non-trivial]

- The trace of operators is the analogue of the integration of functions.

- Tr is linear, $\operatorname{Tr} UAU^* = \operatorname{Tr} A$ for any unitary U and Tr is **operator monotone**, i.e. for $A \leq B$ we clearly have $\operatorname{Tr} A \leq \operatorname{Tr} B$.

- A bounded operator A is called **trace class** iff $\operatorname{Tr}|A| < \infty$. Using the polar decomposition one easily shows that $|\operatorname{Tr} A| \leq \operatorname{Tr}|A|$.

- Trace class operators are compact and they form an ideal within the bounded operators.
- There is a natural norm on the space of the trace class operators, the **trace norm**, defined as
$$\|A\|_{tr} = \operatorname{Tr}|A| = \sum_j \mu_j$$
where μ_j's are the singular values of A (for multiple singuar values the sums are always understood with multiplicity). [It is non-trivial to see that this is indeed a norm]
Obviously
$$\|A\| \leq \|A\|_{tr}$$
- If A is a self-adjoint trace class operator with eigenvalues λ_j, then
$$\operatorname{Tr}|A| = \sum_j |\lambda_j| < \infty, \qquad \operatorname{Tr} A = \sum_j \lambda_j$$
(for multiple eigenvalues the sums are always understood with multiplicity)
- Trace is cyclic: if AB is trace class for some bounded operators A and B then BA is also trace class and
$$\operatorname{Tr} AB = \operatorname{Tr} BA$$
- A compact operator A is called **Hilbert-Schmidt** if A^*A (or, equivalently AA^*) is trace class. The Hilbert-Schmidt norm
$$\|A\|_{HS} = \sqrt{\operatorname{Tr} AA^*} = \sqrt{\operatorname{Tr} A^*A}$$
is indeed a norm on the space of Hilbert-Schmidt operators, moreover this norm comes from a scalar product:
$$\langle A, B\rangle_{HS} := \operatorname{Tr} A^*B$$
that turned the space of Hilbert-Schmidt operators into a Hilbert space. Clearly $\|A\|_{HS} = \|A^*\|_{HS}$
In terms of the singular values, A is Hilbert-Schmidt if and only if $\sum_j \mu_j^2 < \infty$ and
$$\|A\|_{HS}^2 = \sum_j \mu_j^2$$
In particular
$$\|A\| \leq \|A\|_{HS} \leq \|A\|_{tr}$$
so any trace class operator is Hilbert-Schmidt.

- The trace class, the Hilbert-Schmidt and the bounded operators are the natural analogues of the L^1, L^2 and L^∞ Lebesgue spaces for operators. One often uses the notation

$$\|A\|_1 = \|A\|_{tr}, \qquad \|A\|_2 = \|A\|_{HS}$$

The following analogues of Hölder inequalities hold:

$$\|AB\|_1 \leq \|A\| \, \|B\|_1$$

$$\|AB\|_2 \leq \|A\| \, \|B\|_2$$

$$\|AB\|_1 \leq \|A\|_2 \|B\|_2$$

There is a natural definition of L^p spaces (called Schatten-class): a compact operator belongs to the Schatten class of index p ($1 \leq p \leq \infty$) if $\sum_j \mu_j^p < \infty$ and there is an appropriate norm on this space.

So far all these definitions/facts were valid on an arbitrary Hilbert space. The following concept is meaningful only for Hilbert spaces of functions, e.g. $\mathcal{H} = L^2(\mathbf{R}^d)$ or $H^1(\mathbf{R}^d)$. An operator A on a space of functions on $\mathbf{R}^d$ is often given by an operator kernel $a(x, y)$, which is a function on $\mathbf{R}^d \times \mathbf{R}^d$, as

$$(Af)(x) = \int a(x, y) f(y) \mathrm{d}y \tag{6.18}$$

for any function f. Of course this expression as it stands is only formal, one has to ensure that the integral is meaningful. Even not every bounded operator has a kernel, the simplest example is the identity operator. Clearly there is no such function $a(x, y)$ such that

$$(If)(x) = f(x) = \int a(x, y) f(y) \mathrm{d}y$$

Remark. The concept of kernels can be extended to distributions, e.g. one often says that the kernel of the identity operator is $a(x, y) = \delta(x - y)$ since, formally,

$$f(x) = \int \delta(x - y) f(y) \mathrm{d}y$$

This is, however, not quite well defined for any $f(x) \in L^2$ (recall that distributions act only on smooth functions). One can make rigorous mathematical sense of this formula, but we will not need it.

However, from the singular value decomposition for compact operators, one can see that any compact operator A has a kernel in the following sense:

$$(Af)(x) = \sum_j \mu_j \Big(\int \bar{u}_j(y) f(y) \mathrm{d}y \Big) v_j(x) = \int \Big(\sum_j \mu_j \bar{u}_j(y) v_j(x) \Big) f(y) \mathrm{d}y$$

i.e. if we define

$$a(x,y) = \sum_j \mu_j v_j(x) \bar{u}_j(y) \tag{6.19}$$

then (6.18) holds. Of course this sum is only formal and in general defines only a distribution. But we have

Exercise 6.1 *i) Suppose that A is trace class, then the sum in* (6.19) *defines a locally integrable function in both variables, $a(x,y) \in L^1_{loc}(\mathrm{d}x, \mathrm{d}y)$*

ii) Suppose that A is Hilbert-Schmidt, then the sum in (6.19) *defines an $L^2(\mathrm{d}x\mathrm{d}y)$ function. Moreover, we have*

$$\|A\|^2_{HS} = \int |a(x,y)|^2 \mathrm{d}x\mathrm{d}y$$

In these cases we can say that A can be represented as an **integral operator** with **integral kernel** $a(x,y)$.

Remark. The relation between the kernel and the Hilbert-Schmidt norm is very clean. If A is positive and trace class, then

$$\mathrm{Tr}\, A = \int a(x,x) \mathrm{d}x$$

However, one needs a bit care: under the condition, $a(x,y)$ is defined only as an L^1_{loc} function of both variables, in particular, it is defined only for almost every pairs of points (x,y). So a-priori it is meaningless to evaluate $a(x,y)$ on the diagonal. By convention, we define

$$a(x,x) = \sum \lambda_j |v_j(x)|^2,$$

if A has the spectral decomposion (6.15), and by dominated convergence this formula defines an L^1 function $x \to a(x,x)$, which we will *define* to be the diagonal of the operator kernel. If A has a continuous kernel $a(x,y)$ then we can define $a(x,x)$ directly as the diagonal element of the kernel. If, in addition, A is a positive operator, then

$$\mathrm{Tr}\, A = \int a(x,x) \mathrm{d}x$$

holds. The proof is an approximation argument, see e.g. in Reed-Simon Vol III. Section XI.4 (a Lemma to Theorem XI.31).

In other cases there is no explicit formula expressing the relation between various norms of A (e.g. operator norm or trace norm) and $a(x,y)$; only bounds are available.

Exercise 6.2 *Let A be a trace class operator, then the operator norm can be bounded by*

$$\|A\| \leq \Big(ess\sup_x \int |a(x,y)| \mathrm{d}y \Big)^{1/2} \Big(ess\sup_y \int |a(x,y)| \mathrm{d}x \Big)^{1/2}$$

The absolute value of an operator is not related to the absolute value of its kernel, i.e. if $a(x,y)$ is the kernel of A, it does not in general hold that $|a(x,y)|$ is the kernel of $|A|$. In particular, $\mathrm{Tr}\,|A| = \int |a(x,x)| \mathrm{d}x$ is **wrong** (this even does not hold for 2x2 matrices – find a counterexample!)

7 Spectral theorem in general

Here we collect the necessary ingredients for the spectral theorem for general self-adjoint operators.

7.1 Spectral resolution

Definition 7.1 *Given a separable Hilbert space $\mathcal{H}$, a map $E : \mathbf{R} \to \mathcal{B}(\mathcal{H})$ from the real line to the space of bounded operators on $\mathcal{H}$ is called a* **spectral resolution** *if*

- *$E(t)$ is an orthogonal projection*
- *$E(s) \leq E(t)$ for $s \leq t$*
- *$\lim_{\varepsilon \to 0+} E(t+\varepsilon)x = E(t)x$ for any $t \in \mathbf{R}$ and $x \in \mathcal{H}$.*
- *$\lim_{t \to -\infty} E(t)x = 0$, $\lim_{t \to \infty} E(t)x = x$ for any $x \in \mathcal{H}$.*

Notice that E may not be continuous from the left, but $E(t-0) := \lim_{\varepsilon \to 0-} E(t+\varepsilon)$ exists.

Given $f \in \mathcal{H}$, we can consider the function $t \to M^f(t) := \langle E(t)f, f \rangle$ from $\mathbf{R}$ to $\mathbf{R}_+$ which is monotone increasing and continuous from the right. Notice that the limits from the left, $M^f(t-0) := \lim_{\varepsilon \to 0-} M^f(t-\varepsilon)$, exist. Such a function defines a measure μ^f (called the Lebesgue-Stieljes measure) on $\mathbf{R}$ as follows

$$\mu^f[a,b] = M^f(b) - M^f(a-0)$$

This defines the measure of the closed intervals. For open intervals we have

$$\mu^f(a,b) = M^f(b-) - M^f(a)$$

Going through the construction of the Lebesgue measure, one obtains that μ^f can be extended to a measure on the whole Borel sigma algebra of $\mathbf{R}$. It is easy to see that its total mass

$$\int_{\mathbf{R}} \mathrm{d}\mu^f = \|f\|^2 \tag{7.20}$$

Now we can generalize this to **projection-valued measures**. Given a spectral resolution $E(t)$, we define

$$E[a,b] := E(b) - E(a-)$$

and similarly for half closed and open intervals. Notice that $E[a,b]$ is also a projection. Similarly to the construction of the Lebesgue-Stieltjes measure, one can extend the measure E from intervals to any Borel measurable sets, i.e. define $E(\Omega)$ to be a projection for any Ω Borel set, with the usual properties. It is a general fact in measure theory that it is sufficient to check sigma-additivity for disjoint sets, $\Omega_1, \Omega_2, \ldots$, in which case it holds

$$\sum_{j=1}^{\infty} E(\Omega_j) = E\big(\bigcup_{j=1}^{\infty} \Omega_j\big)$$

Here the left hand side is defined as the limit of increasing projections

$$P_N := \sum_{j=1}^{N} E(\Omega_j)$$

as $N \to \infty$. By disjointness of Ω's, P_N is indeed a projection and an increasing set of projections always have a limit in the strong convergence sense (this needs a proof).

Now we can define integration wrt this measure, exactly as we defined Lebesgue integral. For any simple function (or step-function) of the form

$$\phi = \sum_i c_i \mathbf{1}_{I_j}$$

(the sum is finite, $c_j \in \mathbf{C}$ and I_j are disjoint intervals) we set

$$\int_{\mathbf{R}} \phi(\lambda) \mathrm{d}E(\lambda) := \sum_j c_j E(I_j)$$

One has to check that this is well defined. Note that both sides are (bounded) operators on $\mathcal{H}$. Easy computation gives

$$\left\| \int_{\mathbf{R}} \phi(\lambda) \mathrm{d}E(\lambda) f \right\|^2 = \int_{\mathbf{R}} |\phi(\lambda)|^2 d\mu^f(\lambda) \tag{7.21}$$

for any $f \in \mathcal{H}$. Now if $\phi \in L^2(\mathrm{d}\mu^f)$, then there is a sequence of simple functions ϕ_n s.t. $\phi_n \to \phi$ in $L^2(\mathrm{d}\mu^f)$ and this limit defines

$$\int \phi(\lambda) \mathrm{d}E(\lambda) f := \lim_{n\to\infty} \int \phi_n(\lambda) \mathrm{d}E(\lambda) f$$

for any $f \in \mathcal{H}$. To justify this, one needs to check that the r.h.s. is Cauchy in $\mathcal{H}$. The formula (7.21) will hold for any $\phi \in L^2(\mathrm{d}\mu^f)$.

Given a spectral resolution E, we will define a (potentially unbounded) operator $H = H_E$ on $\mathcal{H}$ as follows. The domain is

$$D(H) := \left\{ f \in \mathcal{H} \ : \ \int_{\mathbf{R}} \lambda^2 \mathrm{d}\mu^f(\lambda) < \infty \right\} \tag{7.22}$$

and for any $f \in D(H)$

$$Hf := \int_{\mathbf{R}} \lambda \mathrm{d}E(\lambda) f \tag{7.23}$$

The condition in the definition of $D(H)$ together with (7.21) guarantees that Hf is well defined as an element of $\mathcal{H}$.

This operator is self-adjoint with domain $D(H)$.

Formally it is clear; for the rigorous statement one need the precise definition of the adjoint for unbounded case:

Definition 7.2 *Let the linear operator A be densely defined in $\mathcal{H}$, i.e. its domain $D(A)$ is dense in $\mathcal{H}$. Its adjoint operator A^* is defined by its domain:*

$$D(A^*) := \{ g \in \mathcal{H} \ : \ \exists \widetilde{g} \ \text{ such that } \ \langle g, Af \rangle = \langle \widetilde{g}, f \rangle \ \ \forall f \in D(A) \}$$

and for $g \in D(A^*)$ we set $A^* g := \widetilde{g}$.

The operator A is self-adjoint if $A = A^*$, which also requires that there domains be the same!

An operator A is called **symmetric** if $\langle f, Ag \rangle = \langle A^* f, g \rangle$ for any $f, g \in D(A)$. Notice that $D(A) \subset D(A^*)$. If $D(A) = \mathcal{H}$, then symmetry implies self-adjointness, but in general

symmetry is weaker. But a theorem (Hellinger Toeplitz) states that $D(A) = \mathcal{H}$ for symmetric operators is possible only if A is bouded. Thus unboundedness automatically comes with a domain that is strictly smaller than $\mathcal{H}$ but still dense in it. This shows that there is no way to avoid the domain problem if one deals with unbounded symmetric operators.

Now we come to the main theorem, which is the converse of the construction (7.22)-(7.23):

Theorem 7.3 (Spectral theorem) *Suppose H is self-adjoint. Then there is a unique spectral resolution E (or, equivalently, a projection valued measure $dE(\lambda)$) such that*

$$Hf = \int_{\mathbf{R}} \lambda \mathrm{d}E(\lambda) f$$

for any $f \in D(H)$ (it also contains the statement that the r.h.s. is meaningful for $f \in D(H)$).

Example. Suppose that $\mathcal{H} = \mathbf{C}^N$ and $A = A^*$ is a self-adjoint (=hermitian) matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N$ and eigenvectors $v_1, v_2, \ldots, v_N$. Then the usual spectral theorem asserts that

$$A = \sum_{n=1}^{N} \lambda_n |v_n\rangle\langle v_n| \tag{7.24}$$

We can write this as

$$A = \int \lambda \mathrm{d}E(\lambda)$$

where the spectral resolution is defined as

$$E(t) = \sum_{\lambda_m \leq t} |v_m\rangle\langle v_m|$$

i.e. this is the projection onto the span of the eigenvectors to eigenvalues $\leq$ t. I.e.

$$E(t) = 0 \qquad t < \lambda_1$$

$$E(t) = |v_1\rangle\langle v_1|, \qquad \lambda_1 \leq t < \lambda_2$$

$$E(t) = |v_1\rangle\langle v_1| + |v_2\rangle\langle v_2|, \qquad \lambda_1 \leq t < \lambda_2$$

etc.

7.2 Why are we obsessed by self-adjoint operators?

There are at least two good answers to this question. First is mathematical: because spectral theorem holds for them (and not in general for symmetric operators), and we will see that the spectral theorem is an extremely powerful weapon to do calculations. The second answer is physical: it allows to identify the correct (physical) boundary conditions.

In this section we explain the latter point via a simple example. Suppose the configuration space is the $[0, 2\pi]$ torus with some (so far unspecified) boundary conditions and we wish to define the momentum operator p properly. Of course p acts as $-i\frac{\mathrm{d}d}{\mathrm{d}x}$, but we also have to identify a dense subspace $D(p)$ of $L^2(0, 2\pi)$ so that p is defined on $D(p)$ and $D(p^*) = D(p)$, i.e. p is self-adjoint.

When defining the domain, we have to pay attention to two independent issues. First, a general L^2 function is not differentiable, so we have to impose some *smoothness* requirement. This issue is only a mathematical subtlety here and is not serious. Since we have already introduced the Sobolev spaces and went through the hassle of differentiating "not quite differentiable" functions, we just have to use the $H^1(0, 2\pi)$ space (which is a dense subspace of $L^2(0, 2\pi)$).

The second issue is serious and it is about the boundary conditions. Since we describe the torus, the two endpoints, 0 and 2π are identified, so there is a relation between $f(0)$ and $f(2\pi)$ if f is a physical state. Note that as long as f is only an L^2 function, this issue is irrelevant, since an L^2 function is anyway defined only almost everywhere, so one can always modify its value at one point. But for H^1 functions it is different, we learned that in one dimension, H^1 functions are continuous, in particular it make sense to evaluate them at a point. It would be natural to say that if 0 and 2π are identified, then a reasonable wavefunction f must satisfy $f(0) = f(2\pi)$. But recall the phase is not really a measurable object, so there may be a phase shift between $f(0)$ and $f(2\pi)$. And indeed, you would miss a nontrivial physics (Aharonov-Bohm effect) if you missed this.

We require (at least) two things about the domain that originate from physics:

1) The time evolution should be the shift, i.e. if

$$f_t(x) := e^{-itp} f(x) \tag{7.25}$$

is the time evolution of some initial $f \in L^2(0, 2\pi)$, then we expect $f_t(x) = f(x - t)$. [Why do we expect this? Because this is the evolution generated by the corresponding classical Hamiltonian: $H(x, p) = p$. Then the equations of motions are

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = \partial_p H = 1, \qquad \frac{\mathrm{d}}{\mathrm{d}t}p(t) = -\partial_x H = 0$$

i.e. $x(t) = t + x_0$, $p(t) = p_0$, so the motion in position space is the constant shift.] Notice that e^{-itp} is not (yet) defined, so what we really mean by (7.25) is that f_t solves the corresponding Schrödinger equation:

$$i\partial_t f_t(x) = p f_t(x) = -i\partial_x f_t(x)$$

This means that

$$(\partial_t + \partial_x) f_t(x) = 0$$

and it is trivial to check that $f_t(x) = f(x - t)$ satisfies this equation.

2) The momentum operator is an observable hence the quadratic forms (f, pf) should be real. In particular, p should not have complex eigenvalues (with nonzero real part).

Both issues involve boundary conditions, and they act against each other. First notice that it seems that any complex number λ can be an eigenvalue, simply solve

$$-i\frac{\mathrm{d}}{\mathrm{d}x} f = \lambda f$$

which implies $f(x) = e^{i\lambda x} f(0)$. So unless $f(0) = 0$, any λ is an eigenvalue. Similarly, if you try to solve it from the other end, we get that $f(2\pi) = 0$ must hold. So it seems that to exclude complex eigenvalues, we need $f(0) = f(2\pi) = 0$. But this condition is too restrictive, because the time evolution cannot be defined on such domain (even if initially $f(0) = f(2\pi) = 0$, at a later time the solution f_t, which is a shift of f, will not be zero at the boundary).

So we conclude that if we do not impose any boundary condition (we leave $f(0)$ and $f(2\pi)$ arbitrary, i.e. we just work on $H^1(0, 2\pi)$), then it is too much freedom (we get complex eigenvalues), but if we impose the strongest boundary conditions, $f(0) = f(2\pi) = 0$, then we will have no time evolution. The truth must be somewhere in between.

Here is how it goes. Consider the Hilbert space $\mathcal{H} = L^2(0, 2\pi)$ and recall that $H^1(0, 2\pi)$ is a dense subspace (so far 0 and 2π are not identified). Define the operator A_0 as follows:

$$A_0 = -i\frac{\mathrm{d}}{\mathrm{d}x}, \qquad D(A_0) := \{f \in H^1(0, 2\pi) \ : \ f(0) = f(2\pi) = 0\}$$

This is a small domain, but this makes easy to establish that A_0 is symmetric:

$$(g, A_0 f) = \int \bar{g}(-if') = \int \overline{-ig'} f = (A_0 g, f) \tag{7.26}$$

Here we used integration by parts (which holds for H^1 functions as well, the proof is a standard approximation argument) and the fact that the boundary terms vanish.

Next, we have to find A_0^* based upon the definition of the adjoint. It is a HOMEWORK to check that

$$A_0^* = -i\frac{\mathrm{d}}{\mathrm{d}x}, \qquad D(A_0^*) := H^1(0, 2\pi)$$

I.e. the domain is the largest possible, with no boundary conditions at all. Clearly $D(A_0) \subset D(A_0^*)$ and A_0^* restricted to $D(A_0)$ is A_0, which fact we express by the notation $A_0 \subset A_0^*$.

HOMEWORK: If A and B are densely defined operators and $A \subset B$, then $B^* \subset A^*$

So A_0 is symmetric, but it is "too small", hence its adjoint is "too big". We should try to **extend** A_0 to an operator A, i.e. find an A such that $A_0 \subset A$. Since $A^* \subset A_0^*$, we should try to do it in such a way that $A = A^*$. By extension, A got *increased* compared with A_0 and at the same time A^* got *decreased*, so maybe the gap between A_0 and A_0^* can be closed:

$$A_0 \subset A = A^* \subset A_0^*$$

This goal is called finding **self-adjoint extension of a densely defined symmetric operator**. This may or may not be possible, depending on the original symmetric operator. Moreover, if it is possible, it may not be unique!

Here is one natural candidate for A in our case. Define

$$A = -i\frac{\mathrm{d}}{\mathrm{d}x}, \qquad D(A) = \{f \in H^1(0, 2\pi), \ : \ f(0) = f(2\pi)\}$$

Clearly $A_0 \subset A$ and one has to check that A is symmetric (the boundary terms in the integration by parts in (7.26) still vanish, CHECK). Then CHECK that

$$D(A^*) = D(A)$$

so we indeed found a self-adjoint extension.

Notice that A_0 and A coincide on a dense set (namely on $D(A_0)$), still they behave very differently. It is easy to see that

i) A_0 has no eigenvectors at all. (For, if $A_0 f = \lambda f$, then $f(x) = e^{ix\lambda} f(0)$ but $f(0) = f(2\pi) = 0$ would imply $f \equiv 0$, but the zero vector is not an eigenvector)

ii) A has an orthonormal basis of eigenvectors, namely $\{\frac{1}{\sqrt{2\pi}} e^{inx} \ : \ n \in \mathbf{Z}\}$.

Now we can answer to our original question: what is the good momentum operator? We had three candidates:

$$A_0 \subset A \subset A_0^*$$

and we have seen that A_0 is too small (no dynamics), A_0^* is too large (complex eigenvalues), and A in the middle is the right one.

However, A is not the only possibility. The truth is the following

Theorem 7.4 *All self-adjoint extensions of A_0 are parametrized by a single real parameter $\beta \in [0,1)$, and $A^{(\beta)}$ is defined as*

$$A^{(\beta)} = -i\frac{\mathrm{d}}{\mathrm{d}x}, \qquad D(A^{(\beta)}) = \{f \in H^1(0,2\pi),\ :\ f(0) = e^{2\pi i\beta} f(2\pi)\}.$$

The operator $A^{(\beta)}$ is self-adjoint, it has a complete set of orthonormal eigenfunctions $\{e^{i(n+\beta)x}\ :\ n \in \mathbf{Z}\}$ with eigenvalues $\{n+\beta\ :\ n \in \mathbf{Z}\}$.

The proof is not hard, but we will not do it here. It relies on noticing that $D(A_0)$ is a codimension 2 subspace in $D(A_0^*)$. So if we are looking for an operator A between A_0 and A_0^*, then we only have to specify what happens to two linearly independent vectors.

Physically, $A^{(\beta)}$ is the correct momentum operator if a magnetic flux of size $2\pi\beta$ passes through the torus. Although the magnetic field is supported disjointly from the configuration space (which is a one dimensional wire in a ring), still the electron confined in the ring "feels" the magnetic field. This is the celebrated Aharonov-Bohm effect. It reveals that the topology of the configuration space plays a nontrivial role. In fact, over a topologically nontrivial space, the proper state space of a (spinless) quantum particle is not the L^2 wavefunctions, but L^2-sections of a $U(1)$-bundle over the configuration space.

Back to self-adjoint extensions, in general, there is a complete theory which tells us if there is a self-adjoint extension of a densely defined symmetric operator A_0 and how many. The answer is not surprising: if the codimension of $D(A_0)$ as a subspace of $D(A_0^*)$ is odd, then there is no extension. If this codimension is even, say $2n$, then there is an n-parameter family of extensions (this includes the $n = \infty$ case).

There is however one very important case, when all these complications are absent. The following theorem by Friedrichs states that for **semibounded** operators, there is a unique self-adjoint extension (the proof is not very hard but it requires some nontrivial preparation):

Theorem 7.5 *Let H be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ and assume that H is semibounded, i.e. there is a finite constant C such that*

$$(f, Hf) \geq -C\|f\|^2, \qquad \forall\ f \in D(H) \tag{7.27}$$

(we can assume that C denotes the smallest such constant). Then there exists a self-adjoint extension that preserves the semiboundedness with the same lower bound $-C$ and this extension is (essentially) unique.

(The word "essentially" refers to an extra technical condition that the domain of the extension does not exceed the maximal form domain, a concept that we did not introduce here, but this requirement is natural.)

In applications, H is the Hamiltonian and the semiboundedness corresponds to the stability of the system. For example, if $H = -\Delta + V$, then (7.27) is implied (simple density argument) by the semiboundedness of the corresponding quadratic form, i.e. by

$$\int |\nabla f|^2 + \int V|f|^2 \geq -C\|f\|^2$$

and it is sufficient to check it on a dense subset of $D(H)$, in most cases for $f \in C_0^\infty(\mathbf{R}^d)$ suffices. This is one (main) reason why stability of H is so important.

7.3 Functional calculus

Once we have a representation of a self-adjoint operator as an integral we can easily define functions of operators. Taking polynomials of an operator is easy, e.g. A^2 is just repeated application of A, so if there is no domain issue, then $(A^2)f := A(Af)$, trivially. Simple check shows that in the case of hermitian matrices, $A = A^*$ of the form (7.24), we have

$$A^2 = \sum_{n=1}^{N} \lambda_n^2 |v_n\rangle\langle v_n| = \int \lambda^2 \mathrm{d}\ E(\lambda)$$

i.e. the spectral projections remain the same, but the eigenvalues get squared, or alternatively, we integrate the function λ^2 instead of λ against the projection valued measure.

Clearly this procedure works for any bounded function. Given $F : \mathbf{R} \to \mathbf{C}$ a bounded measurable function (actually it is sufficient that F is defined on $\sigma(H)$, the spectrum of H), we set

$$F(H) := \int F(\lambda)\mathrm{d}E(\lambda)$$

This is a bounded linear operator and it satisfies all the nice properties (it is a C^*-algebra homomorphism between bounded functions on $\sigma(H)$ and bounded operators). E.g.

$$F(H) + G(H) = (F+G)(H), \qquad F(H)G(H) = (F\cdot G)(H), \qquad F(H)^* = (\bar{F})(H)$$

where bar denotes the complex conjugate. In particular, one can define e^{-itH} in this way.

The very good news is that all these manipulations go through to unbounded self-adjoint operators. *Once self-adjointness if established, the rest comes for (almost) free!* There is always a domain issue, but the theory takes care of it automatically. Let me just show what I mean by that through two easy examples.

The first example is to show that the spectrum of a self-adjoint operator H is real, $\sigma(H) \subset \mathbf{R}$. To show this, enough to check that any $z \in \mathbf{C} \setminus \mathbf{R}$ is in the resolvent set, i.e. that $(H-z)^{-1}$ is bounded. But indeed by (7.21) and (7.20), we have

$$\left\| \frac{1}{H-z} f \right\|^2 = \int_{\mathbf{R}} \frac{1}{|\lambda - z|^2} \mathrm{d}\mu^f(\lambda) \leq \frac{1}{|Imz|^2} \int_{\mathbf{R}} \mathrm{d}\mu^f(\lambda) = \frac{1}{|Imz|^2} \|f\|^2$$

for any $f \in \mathcal{H}$, thus

$$\left\| \frac{1}{H-z} \right\| \leq \frac{1}{|Imz|}$$

In the second example, we suppose that H is an unbounded self-adjoint operator on $\mathcal{H}$ and let F and G be (possibly) unbounded functions. In analogy with (7.22), it turns out that

$$D(F(H)) := \left\{ f \in \mathcal{H} \ : \ \int |F(\lambda)|^2 \mathrm{d}\mu^f(\lambda) < \infty \right\}$$

This is because $f \in D(F(H))$ means that $F(H)f \in L^2$, but the spectral theorem and (7.21) show that

$$\|F(H)f\|^2 = \left\| \int_{\mathbf{R}} F(\lambda) \mathrm{d}E(\lambda) f \right\|^2 = \int_{\mathbf{R}} |F(\lambda)|^2 \mathrm{d}\mu^f(\lambda)$$

Similarly one can define $G(H)$ and its domain. Now suppose we want to define the product operator $F(H)G(H)$. It should hold that

$$F(H)G(H) = (F \cdot G)(H)$$

also in the unbounded case. But now there is a domain issue and the natural domains of the two sides might not be the same. But they are: the natural domain of $F(H)G(H)$ is

$$D(F(H)G(H)) = \left\{ f \in D(G(H)) \ : \ G(H)f \in D(F(H)) \right\}$$

The first condition says that

$$\int |G(\lambda)|^2 \mathrm{d}\mu^f(\lambda) < \infty \tag{7.28}$$

The second condition requires

$$\int |F(\lambda)|^2 \mathrm{d}\mu^{G(H)f}(\lambda) < \infty \tag{7.29}$$

We will check below that

$$\mathrm{d}\mu^{G(H)f}(\lambda) = |G(\lambda)|^2 \mathrm{d}\mu^f(\lambda) \tag{7.30}$$

so (7.29) means

$$\int |F(\lambda)|^2 |G(\lambda)|^2 \mathrm{d}\mu^f(\lambda) = \int |(F \cdot G)(\lambda)|^2 \mathrm{d}\mu^f(\lambda) < \infty$$

which is the condition for $f \in D((F \cdot G)(H))$. Notice however that condition (7.28) is not present when one considers the operator $(F \cdot G)(H)$, so in fact we proved that

$$F(H)G(H) \subset (F \cdot G)(H)$$

and they may not be equal. However, the source of the discrepancy is very natural, since $F(H)G(H)$ acting on a function requires an intermediate calculation that may be more restrictive. For example we have

$$H^{-1}H = I$$

where the identity on the r.h.s can act on any function, while the l.h.s can be computed only on $D(H)$.

Finally, we check (7.30). It is enough to check that the distribution functions of these two measures are the same, i.e. we compute for any $t \in \mathbf{R}$ by using (7.21)

$$\int_{-\infty}^{t} \mathrm{d}\mu^{G(H)f}(\lambda) = \Big\langle E(t)G(H)f, E(t)G(H)f \Big\rangle = \int_{\mathbf{R}} \big|\mathbf{1}(\lambda \leq t)G(\lambda)\big|^2 \mathrm{d}\mu^f(\lambda) = \int_{-\infty}^{t} |G(\lambda)|^2 \mathrm{d}\mu^f(\lambda).$$

7.4 Spectrum and spectral types

The spectrum of a self-adjoint H can be identified from the spectral representation E of H, namely one can prove that $\lambda \in \sigma(H)$ iff for any $\varepsilon > 0$ we have

$$E(\lambda + \varepsilon) - E(\lambda - \varepsilon) \neq 0$$

The point spectrum and continuous spectrum are identified as before, but now we can even define spectral subspaces. Given $H = H^*$, set

$$\mathcal{H}_p = \overline{\text{Span (eigenvectors)}}$$

and

$$\mathcal{H}_c := (\mathcal{H}_p)^{\perp}$$

The continuous spectrum further splits into two parts, singular continuous and absolute continuous parts that are defined as follows

$$\mathcal{H}_{sc} := \Big\{ f \in \mathcal{H}_c \ : \ \exists S \subset \mathbf{R},\ E(S)f = f,\ |S| = 0 \Big\}$$

Equivalently:

$$\mathcal{H}_{sc} := \Big\{ f \in \mathcal{H} \ : \ \mathrm{d}\mu^f \ \text{ is singular continuous} \Big\}$$

(recall the definition of $\mathrm{d}\mu^f$ from Section 7.1). Similarly

$$\mathcal{H}_{ac} := \Big\{ f \in \mathcal{H} \ : \ \mathrm{d}\mu^f \ \text{ is absolutely continuous} \Big\}$$

Recall that absolutely continuous means that the measure is given by an L^1 function, i.e. there is a function $\psi^f \in L^1(\mathbf{R})$ such that

$$\mu^f(\Omega) = \int_\Omega \psi^f(t)\mathrm{d}t$$

for any measurable $\Omega \subset \mathbf{R}$.

It is a (nontrivial) fact that these subspaces are orthogonal, i.e.

$$\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_{sc} \oplus \mathcal{H}_{ac}$$

is an orthogonal decomposition.

7.5 Dynamics and spectrum

The various spectral types manifest themselves in the behavior of the time evolution e^{-itH}. Clearly if f is an eigenvector, $Hf = \lambda f$, then $e^{-itH}f = e^{-it\lambda}f$ for any $t \in \mathbf{R}$, in particular $e^{-itH}f$ will remain parallel with f.

If $f \in \mathcal{H}_{ac}$, then

$$\lim_{|t|\to\infty} \langle e^{-itH}f, f\rangle = \lim_{|t|\to\infty} \int_{\mathbf{R}} e^{-it\lambda}\mathrm{d}\mu^f(t) = 0 \tag{7.31}$$

by the Riemann-Lebesgue lemma (Fourier transform of an L^1 function decays at infinity). This means that after a long time evolution the state will turn orthogonal to its original.

Finally, the continuous spectrum (in contrast to the point spectrum) is characterized by the fact that the overlap of $e^{-itH}f$ with f will vanish in a time-averaged sense:

$$\frac{1}{T}\int_0^T |\langle e^{-itH}f, f\rangle|^2 \mathrm{d}t \to 0, \qquad f \in \mathcal{H}_c, \tag{7.32}$$

as $T \to \infty$. The proof relies on Wiener theorem that is an easy exercise:

Theorem 7.6 *Let μ be a finite complex measure on $\mathbf{R}$ and let*

$$\widehat{\mu}(t) := \int e^{-it\lambda} \mathrm{d}\mu(\lambda)$$

be its Fourier transform. Then

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T |\widehat{\mu}(t)|^2 \mathrm{d} = \sum_{\lambda\in\mathbf{R}} |\mu(\lambda)|^2$$

In fact, the result (7.32) extends to a the more general case:

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T |\langle e^{-itH} f, g\rangle|^2 \mathrm{d}t = 0, \qquad f \in \mathcal{H}_c, \quad g \in \mathcal{H}. \tag{7.33}$$

This is the rank-one version of the RAGE theorem:

Theorem 7.7 *Let H be self-adjoint and suppose that K is relatively compact wrt. H (this means that $K(H-z)^{-1}$ is compact for any $z \in \mathbf{C} \setminus \mathbf{R}$). Then*

$$\lim_{t\to\infty} \|Ke^{-itH} f\| = 0 \qquad \forall\, f \in \mathcal{H}_{ac}$$

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \|Ke^{-itH} f\| \mathrm{d}t = 0 \qquad \forall\, f \in \mathcal{H}_c$$

The proof is an approximation argument, once we know it for K rank one, we will know it for finite linear combinations, and any compact operator can be approximated (in norm sense) by finite rank operators. This proves the case when K is compact. The extension to relative compact K requires a little extra argument.

In particular, it is easy to see that the multiplication by the characteristic function of a compact set $B \in \mathbf{R}^3$ is relatively compact wrt $-\Delta$ and also $-\Delta + V$ under reasonable conditions on V. Thus we obtain the RAGE theorem used in scattering theory, expressing that scattering states leave any compact domain B:

$$\lim_{t\to\infty} \int_B |e^{-itH} f|^2 = 0 \qquad \forall\, f \in \mathcal{H}_{ac}$$

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \int_B |e^{-itH} f|^2 \mathrm{d}t = 0 \qquad \forall\, f \in \mathcal{H}_c.$$

8 Density matrices

So far we described the state of a quantum system by (normalized) wave functions $\psi \in L^2(\mathbf{R}^{dN})$ (or, if with spin, then $\psi \in L^2(\mathbf{R}^{dN}, \mathbf{C}^Q)$ with $Q = \prod_i q_i$), and recall that we had a slight ambiguity: multiplication by a constant phase does not change the physical state (although it changes the wave function in a trivial way). Instead of ψ, we can think of the quantum state as a rank-one orthogonal projection in the Hilbert space, that projects onto the one-dimensional space spanned by ψ:

$$\Gamma_\psi : \mathcal{H} \to \mathcal{H}, \qquad \Gamma_\psi \phi = \langle \psi, \phi \rangle \psi$$

The physics notation is $\Gamma_\psi = |\psi\rangle\langle\psi|$. Note that this idea removes the ambiguity with the constant phase multiple.

Obviously Γ_ψ is

- self-adjoint, $\Gamma_\psi^* = \Gamma_\psi$,
- positive semidefinite, $\langle \phi, \Gamma_\psi \phi \rangle \geq 0$, $\forall \phi \in \mathcal{H}$, denoted as

$$\Gamma_\psi \geq 0$$

- is trace class with $\operatorname{Tr} \Gamma_\psi = 1$.
- idempotent: $\Gamma_\psi^2 = \Gamma_\psi$

The rank-one projections Γ_ψ are also called **pure states** or **pure state density matrices**. [The word "matrix" is a bit misleading since these are operators in an infinite dimensional space.] The pure states are equivalent to wave functions (modulo the irrelevant phase ambiguity). The energy of the wave function can be expressed as

$$\operatorname{Tr} H\Gamma_\psi = \langle \psi, H\psi \rangle$$

and the Schrödinger time evolution is expressed by a commutator:

$$i\partial_t \psi_t = H\psi_t \quad \Longleftrightarrow \quad i\partial_t \Gamma_{\psi_t} = [H, \Gamma_{\psi_t}]$$

where $[A, B] = AB - BA$. These expressions are formal for the moment, since neither the trace nor the commutator has been defined for unbounded operators.

There are more general possible states of a quantum system than the ones described by pure states (or wave functions). Suppose we want to describe a statistical state, where the particle in state ψ_1 with a certain probability p and in state ψ_2 with probability $1 - p$ with $\psi_1 \perp \psi_2$.

The correct description is **not** the linear combination of these two states, $\psi = p\psi_1 + (1-p)\psi_2$. There are several reasons why this naive attempt is not correct. First $\|\psi\|_2^2 = p^2 + (1-p)^2 < 1$. This could be remedied by taking $\psi = \sqrt{p}\psi_1 + \sqrt{1-p}\psi_2$. Second, more fundamentally, ψ itself is a wave function (pure state) and there is no way to recover ψ_1, ψ_2 or p from ψ, so we completely lose the information that the description supposed to carry.

The correct description of such a state is the **density matrix**

$$\Gamma = p\Gamma_{\psi_1} + (1-p)\Gamma_{\psi_2}$$

which is an operator on Γ. Obviously

$$0 \leq \Gamma \leq I, \qquad \operatorname{Tr}\Gamma = 1 \tag{8.34}$$

Note that $\Gamma \leq I$ follows from $\Gamma \geq 0$ and $\operatorname{Tr}\Gamma = 1$. Clearly p and the one dimensional spaces generated by ψ_1 and ψ_2 can be recovered from Γ by the spectral decomposition.

In full generality, we have:

Definition 8.1 *A non-negative operator $\Gamma \geq 0$ on $\mathcal{H}$ with unit trace, $Tr\Gamma = 1$, is called* **density matrix**. *Density matrices describe* **(mixed) quantum states**.

Any density matrix is trace class, hence compact, thus it has a spectral decomposition

$$\Gamma = \sum_j \lambda_j \Gamma_{\psi_j}$$

with non-negative eigenvalues that add up to one: $\sum_j \lambda_j = 1$ and with normalized eigenvectors ψ_j. Thus any density matrix is a convex linear combination of pure states: the eigenvalues are interpreted as statistical weights (probabilities) that the system is in the pure state ψ_j. Moreover, the set of density matrices is convex, i.e. convex linear combination of density matrices is a density matrix. The extremal points of this convex set are the pure states.

Recall the general definition of the operator kernel of a trace class operator from the end of Section 6. Since Γ is a trace class operator, it has an operator kernel, denoted also by Γ but indicating the variables, i.e. $\Gamma(x,y)$ is defined as

$$\Gamma(x,y) = \sum_j \lambda_j \psi_j(x)\bar{\psi}_j(y)$$

and it is a locally integrable function. The diagonal element of Γ is *defined* as

$$\Gamma(x,x) := \sum_j \lambda_j |\psi_j(x)|^2$$

which is an L^1 function and

$$\operatorname{Tr}\Gamma = \int \Gamma(x,x)\mathrm{d}x = \sum_j \lambda_j$$

If we take spins into account, then the space variable x, y etc. should be replaced by the composite variable $z = (x, \sigma)$, etc.

8.1 Outlook: why density matrices are important

Density matrices typically arise in a situation when one describes a subsystem. Suppose we have a particle with position x in a heat bath of other particles with position $y_1, y_2, ...y_N$. The correct wave function of the system is a function $\Psi(x, y_1, \dots y_N)$ of $N+1$ variables. In many cases we want to observe only the distinguished particle, i.e. we want to make measurements with observables acting only on the x variable, e.g. $O = O(x)$ where O is a function. Then we compute

$$\langle \Psi, O\Psi\rangle = \int O(x)|\Psi(x, y_1, \dots y_N)|^2 \mathrm{d}x\mathrm{d}y_1 \dots \mathrm{d}y_N$$

or, more generally, O is an operator with kernel $O(x, x')$ (still acting on x only):

$$\langle \Psi, O\Psi\rangle = \int O(x, x')\bar{\Psi}(x', y_1, \dots y_N)\Psi(x, y_1, \dots y_N)\mathrm{d}x\mathrm{d}x'\mathrm{d}y_1 \dots \mathrm{d}y_N$$

We can define a density matrix as

$$\gamma(x, x') := \int \Psi(x, y_1, \dots y_N)\bar{\Psi}(x', y_1, \dots y_N)\mathrm{d}y_1 \dots \mathrm{d}y_N \tag{8.35}$$

(which is the one particle reduced density matrix of Ψ, see next section, there it will be denoted by $\gamma^{(1)}$ or $\gamma^{(1)}_\Psi$). The operation (8.35) can also be written as

$$\gamma(x, x') := \int \Gamma_\Psi(x, y_1, \dots y_N; x', y_1, \dots y_N)\mathrm{d}y_1 \dots \mathrm{d}y_N$$

i.e. taking the partial trace of Γ_Ψ with respect to all but the first variable. The notation is

$$\gamma = \operatorname{Tr}_{y_1,\dots y_N}\Gamma.$$

It is easy to see that $\gamma \geq 0$, $\operatorname{Tr}\gamma = 1$ (next section for the normalization convention), but in general γ is not a pure state. Nevertheless

$$\langle \Psi, O\Psi\rangle = \int O(x, x')\gamma(x, x')\mathrm{d}x\mathrm{d}x' = \operatorname{Tr} O^*\gamma$$

so the expectation value of the observable O can be computed from γ. It is therefore sufficient to know γ instead of Ψ, and γ is a much simpler object (since it is a one-particle object).

The key question is however, whether γ has a self-consistent evolution or not, i.e. whether it is really sufficient to know γ initially at $t = 0$ to compute γ_t at a later time t. We have a Hamiltonian H describing the time evolution of the $N + 1$ particles:

$$i\partial_t \Psi_t = H\psi_t$$

or, equivalently,

$$i\partial_t \Gamma_t = [H, \Gamma_t] \tag{8.36}$$

In general it is not true that $\gamma = \gamma_t$ evolves according to a one-particle hamiltonian h, since the interaction with the other particles $y_1, \dots y_N$ influences the evolution of x. In other words, if one takes the partial trace of (8.36), we get

$$i\partial_t \gamma_t = \mathrm{Tr}_{y_1,\dots y_N}[H, \Gamma_t]$$

but the right hand side **cannot**, in general, be written as

$$\mathrm{Tr}_{y_1,\dots y_N}[H, \Gamma_t] = [h, \gamma_t] \tag{8.37}$$

for some suitable one-particle Hamiltonian h. But in some cases (e.g. when H has no interaction between x and the y's, or sometimes in some limiting regimes, such as semiclassical or mean-field limits), the equation (8.37) holds, and then it is sufficient to solve the one-particle Schrödinger equation

$$i\partial_t \gamma_t = [h, \gamma_t]$$

to find the expected value of the observable $\mathrm{Tr}\, O^* \gamma_t$ at later times. This is one possible justification why one would like to extend quantum mechanics to mixed states.

Exercise 8.2 *Let h, g be Hamilton operators on the one-particle Hilbert space $\mathcal{H}$. Let $H = h \otimes I + I \otimes g$ be a non-interacting Hamiltonian acting on the two-particle Hilbert space $\mathcal{H} \otimes \mathcal{H}$. Let Γ be a two-particle density matrix and $\gamma = Tr_y \Gamma$ be its marginal reduced density matrix on the x variable. Prove that if $\Gamma = \Gamma_t$ is the solution to the Schrödinger evolution*

$$i\partial_t \Gamma_t = [H, \Gamma]$$

then

$$i\partial_t \gamma_t = [h, \gamma]$$

Of course so far this is only a tautology; for non-interacting systems we do not expect that we need to know anything about the other particles to predict the evolution of the x-particle, say.

But there are many interacting systems (typically mean-field systems), where in certain asymptotic regime the description with one particle density matrices is *approximately* correct. This usually needs a nontrivial mathematical derivation. Here is one theorem of this type:

Theorem 8.3 (Derivation of the Hartree equation) *Consider N bosons in d dimensions described by the Hamiltonian*

$$H = \sum_{j=1}^{N} -\Delta_j + \frac{1}{N}\sum_{i<j} U(x_i - x_j)$$

with some two body potential U. For simplicity, assume that U is bounded. Note the prefactor $1/N$, i.e. each particle interacts with each other, but the interaction is substantially weakened. Suppose that the initial state is a product, i.e. $\Psi_0^{(N)} = \bigotimes_1^N f_0$ with some single particle wavefunction $f_0 \in L^2(\mathbf{R}^d)$. Let Ψ_t be the solution to the (N-body) Schrödinger equation

$$i\partial_t \Psi_t^{(N)} = H\Psi_t^{(N)} \tag{8.38}$$

with initial condition $\Psi_{t=0}^{(N)} = \Psi_0$. Let $\gamma_{N,t}^{(1)} := \gamma_{\Psi_t^{(N)}}^{(1)}$ be the one particle reduced density matrix of the solution. Then the limit

$$\lim_{N\to\infty} \gamma_{N,t}^{(1)} = \gamma_t^{(1)}$$

exists (in the trace norm topology), the limit is a one particle density matrix, $\tilde{r}\gamma_t^{(1)} = 1$, and it satisfies the **Hartree equation**

$$i\partial_t \gamma_t^{(1)} = \Big[-\Delta + U \star \varrho_t, \gamma^{(1)} \Big] \tag{8.39}$$

where $\varrho_t(x) = \gamma_t^{(1)}(x,x)$ is the density.

The significance of such theorems is that it allows to predict the time evolution of certain observables (namely those ones which depend only on one variable, i.e. they can be computed via the one particle density matrix) without solving the N-body Schrödinger equation (which is hard!). Instead of solving a PDE in $N \approx 10^{23}$ variables, we just have to solve an equation (8.39) in one variable. The price we pay is that the new equation is for density matrices (instead of wave functions) and that it is nonlinear (it is quadratic in γ). Furthermore, it

holds only in a limiting regime, i.e. it is not a *first principle* equation, but it is only an *effective equation*.

Note that in many physics textbooks these effective equations are presented as the starting point of the analysis. Actually many famous equations (like Gross-Pitaevskii equation for the Bose-Einstein condensate, the BCS and the Ginzburg-Landau equations for superconductivity etc.) are of this type. For pragmatical point of view this is fine, but you should be aware that there is always a "derivation" behind these effective equations, that goes back to the honest Schrödinger theory. The mathematically rigorous derivation is typically very hard and has been done only in a few cases.

8.2 H^1 density matrices and the energy

We say that Γ is a H^1-density matrix if for all eigenfunctions $\psi_j \in H^1(\mathbf{R}^{dN})$ and if

$$\sum_j \lambda_j \|\nabla \psi_j\|_2^2 < \infty \tag{8.40}$$

Formally this sum is just $\operatorname{Tr}(-\Delta)\Gamma$, since

$$\operatorname{Tr}(-\Delta)\Gamma = \sum_j \langle \psi_j, (-\Delta)\Gamma\psi_j\rangle = \sum_j \lambda_j \langle \psi_j, (-\Delta)\psi_j\rangle = \sum_j \lambda_j \|\nabla\psi_j\|^2$$

using that $\Gamma\psi_j = \lambda_j\psi_j$. Notice that both $-\Delta$ and Γ are non-negative operators, so their trace can be defined for any Γ density matrix by the formula above; the trace is always non-negative, but it may be infinite.

The trace is like an integration: similarly to the integral of a positive function that may be infinite, the trace of a positive operator can always be defined, but it may be infinite. Notice however, that the product of two positive operator is typically not positive, e.g. $(-\Delta)\Gamma$ is not positive (even not self-adjoint). But one can use the cyclicity of the trace after having written $(-\Delta) = p^2$ (recall $p = -i\nabla$), i.e.

$$\operatorname{Tr}(-\Delta)\Gamma = \operatorname{Tr} p\Gamma p$$

and now clearly $p\Gamma p$ is a positive operator.

In principle here the cyclicity is formally applied, and you may worry about domain questions. The rule of thumb is that as long as one has a finite control of the form (8.40), all these formal steps are allowed. The reason is that each ψ_j can be arbitrarily well approximated in H^1 sense by C_0^∞ functions. For such functions, and taking finite truncations of the sum, everything is rigorous. Then one can remove the approximation by using the uniform

upper bound. This is the operator-version of the "standard approximation argument" that we learned about functions.

We can similarly define the expected value of the potential energy. If $U(x_1, \dots x_N)$ is a real function, then

$$\operatorname{Tr} U\Gamma = \sum_j \langle \psi_j, U\Gamma\psi_j\rangle = \sum_j \lambda_j \langle \psi_j, U\psi_j\rangle = \sum_j \lambda_j \int U|\psi_j|^2$$

again with the understanding that the left hand side is defined if the right hand side make sense.

Similarly we can define the expectation value of the Hamiltonian $H = \sum_j(-\Delta_j) + U(x_1, \dots x_N)$ in the state Γ as

$$\operatorname{Tr} H\Gamma = \operatorname{Tr} \Gamma H := \sum_j \lambda_j \mathcal{E}(\psi_j) \tag{8.41}$$

where, recall that

$$\mathcal{E}(\psi) = \int |\nabla\psi|^2 + U|\psi|^2$$

Although $\operatorname{Tr} H\Gamma$ is not defined a-priori, we can use the right hand side of the definition (8.41) as long as $\sum_j \lambda_j |\mathcal{E}(\psi_j)|$ is finite. With the same token we can define $\operatorname{Tr} A\Gamma$ for any observable (self-adjoint operator) A if the eigenfunctions ψ_j in the spectral decomposition of $\Gamma = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$ lie in the domain of the quadratic form of A and $\sum_j \lambda_j |\langle\psi_j, A\psi_j\rangle| < \infty$. [We have not defined the domain of a quadratic form of an unbounded self-adjoint operator, but this has the same relation to A as the Dirichlet integral $\int |\nabla\psi|^2$ has with $-\Delta$.]

From (8.41) it immediately follows that

$$\inf\{\mathcal{E}(\psi) \ : \ \|\psi\|_2 = 1\} = \inf\{\mathcal{E}(\Gamma) \ : \ \Gamma \text{ is a density matrix}\} \tag{8.42}$$

This means that although the density matrices are more general than wave functions (equivalent with rank-one density matrices), as far as the ground state energy is concerned, we do not get lower energy if we apply the variational principle for a bigger set of objects. There are several advantages of considering the problem in the r.h.s. of (8.42). First, the functional $\Gamma \to \mathcal{E}(\Gamma)$ is linear. Second, the minimization is over a convex set, since the constraints on Γ, namely $\Gamma \geq 0$ and $\tilde{r}\Gamma = 1$ are convex constraints (determine a convex set in the space of operators). The convexity could be restored for the problem in the l.h.s, namely, it is easy to prove (CHECK) that

$$\inf\{\mathcal{E}(\psi) \ : \ \|\psi\|_2 = 1\} = \inf\{\mathcal{E}(\psi) \ : \ \|\psi\|_2 \leq 1\} =$$

i.e. the constraint ψ being on the unit sphere of the Hilbert space (which is not a convex set) can be relaxed to require ψ being in the unit ball, which is convex. But the fact that $\psi \to \mathcal{E}(\psi)$ is quadratic is inherent.

According to the symmetry type of the underlying Hilbert space (symmetric or antisymmetric subspace), the density matrices can also be symmetric (bosonic) or antisymmetric (fermionic). The symmetry type of a density matrix is not the same as the symmetry of the operator kernel $\Gamma(x, x')$ (or from $\Gamma(z, z')$ if spins are included). For example, if $\Gamma = \Gamma_\psi$, then its kernel is

$$\Gamma(x_1, x_2, \dots x_N, x'_1, x'_2, \dots x'_N) = \psi(x_1, x_2, \dots x_N)\bar{\psi}(x'_1, x'_2, \dots x'_N)$$

If we interchange, say, the variables 1 and 2, then we get

$$\Gamma(x_1, x_2, \dots x_N, x'_1, x'_2, \dots x'_N) = \Gamma(x_2, x_1, \dots x_N, x'_2, x'_1, \dots x'_N)$$

both in case of fermions and bosons. [Important: Note that both x_1, x_2 and x'_1, x'_2 have to be simultaneously permuted.]. Thus density matrices, as functions of $N + N$ variables, are always symmetric. To see whether they are fermionic or bosonic density matrices, one has to write up their spectral decomposition. If all eigenfunctions are symmetric (antisymmetric), then the density matrix maps the symmetric (antisymmetric) subspace into itself and then the density matrix has a definite symmetry type, otherwise not.

Alternatively, one can test whether $\Gamma(x, x')$ is symmetric (antisymmetric) w.r.t permuting only among the x or only among the x' variables. This is a non-physical operation (since mixes up particle variables), but it can be used as a test. E.g. if we require that ($\sigma = 1$ stands for bosons, $\sigma = -1$ for fermions)

$$\begin{aligned}\Gamma(x_1, x_2, \dots x_N; x_1,' x'_2, \dots x'_N) &= (-1)^\sigma \Gamma(x_2, x_1, \dots x_N; x_1,' x'_2, \dots x'_N) \\ &= (-1)^\sigma \Gamma(x_1, x_2, \dots x_N; x_2,' x'_1, \dots x'_N)\end{aligned}$$

and similar relations hold for interchanging any two indices (i, j) instead of $(1, 2)$, then Γ is a bosonic ($\sigma = 1$) or fermionic ($\sigma = -1$) density matrix.

9 Reduced density matrices

Definition 9.1 *Let Γ be a symmetric or antisymmetric N-particle density matrix and let $1 \le k \le N$. The* **k-particle reduced density matrix (or k-particle marginal)** *of Γ is defined as*

$$\gamma^{(k)}(z_1, \dots z_k; z'_1, \dots z'_k) = \frac{N!}{(N-k)!} \int \Gamma(z_1, \dots z_k, z_{k+1}, \dots z_N; z'_1, \dots z'_k, z_{k+1}, \dots z_N) \mathrm{d}z_{k+1} \dots \mathrm{d}z_N$$

in other words, we fix the first $k + k$ variables in the kernel Γ, and set the other $N - k$ variables equal and integrate them out. For the precise meaning, we have to write Γ into its eigenfunction expansion.

Remarks.

i) This formula defines the kernel of an operator $\gamma^{(k)}$ that acts on the k-particle bosonic or fermionic space (check that $\gamma^{(k)}$ leaves these spaces invariant if Γ had the same property on the N-body level).

ii) The procedure of fixing $k+k$ variables, setting the rest equal and integrate out is called **taking the partial trace** (note that for $k = 0$ it would indeed correspond to taking the "full" trace). We will not need this concept now, so we will not define it precisely.

iii) The prefactor is a convention: with this normalization

$$\operatorname{Tr} \gamma^{(k)} = \frac{N!}{(N-k)!} \tag{9.43}$$

It reflects all possible combinatorics in the general case. If Γ were not symmetric, then the proper definition of $\gamma^{(k)}$ would be to take all possible k-element subsets of the index set and also symmetrize with respect to the k variables. This would give $\frac{N!}{(N-k)!}$ terms. By symmetry, all these terms are the same, so we can just decide to integrate out the last $N-k$ variables, not symmetrize in the first k variables and account for the combinatorics via the prefactor.

If you compare Definition 9.1 with (8.35) from the previous section, then you see that they differ by the normalization. There are two concurring conventions in the literature; either all $\gamma^{(k)}$ is normalized to have trace 1,

$$\operatorname{Tr} \gamma^{(k)} = 1$$

or (9.43) holds. The former has an advantage in situations when $N \to \infty$ limit is directly considered (e.g. in mean-field limit of interacting systems), since the convention keeps the sequence of density matrices, e.g. $\gamma^{(1)}_{\Psi_N}$, of N-particle wave functions, uniformly bounded (in trace norm), therefore subsequential compactness can be extracted (there is an operator version of Banach-Alaoglu theorem). The normalization (9.43) is better when the explicit N-dependence is relevant, e.g. $\operatorname{Tr} \gamma^{(1)} = N$ directly expresses the number of particles. In this course we will follow the convention (9.43) since it is more suited to our purposes.

iv) The diagonal element of the one-particle reduced density matrix of a pure state $\Gamma = |\psi\rangle\langle\psi|$ is just the one-particle density defined in (1.2):

$$\gamma^{(1)}(x,x) = \varrho(x)$$

An important observation is that $\gamma^{(k)}$ is positive semi-definite:

Exercise 9.2 *Using the spectral decomposition of* Γ*, prove that* $\langle\phi, \gamma^{(k)}\phi\rangle \geq 0$ *for any function* $\phi \in L^2(\mathbf{R}^{kd}; \mathbf{C}^q)$

Exercise 9.3 *i) Let* $\Gamma = \Gamma_\psi$ *be a bosonic pure state with* $\psi = \otimes_1^N f$*. Compute* $\gamma^{(k)}$*. In particular, prove that*

$$\gamma^{(k)} = \otimes_{j=1}^k \gamma^{(1)}$$

i.e.

$$\gamma^{(k)}(z_1, \ldots, z_k; z_1', \ldots, z_k') = \prod_{j=1}^k \gamma^{(1)}(z_j, z_j')$$

ii) Let $\Gamma = \Gamma_\psi$ *be a fermionic pure state with* $\psi = f_1 \wedge f_2 \wedge \ldots \wedge f_N$ *being a Slater determinant of orthonormal functions. Compute* $\gamma^{(k)}$*. In particular, prove that*

$$\gamma^{(1)}(z, z') = \sum_{j=1}^N f_j(z)\bar{f}_j(z') \tag{9.44}$$

and for the diagonal element of the two particle reduced density matrix we have

$$\gamma^{(2)}(z_1, z_2; z_1, z_2) = \gamma^{(1)}(z_1, z_1)\gamma^{(1)}(z_2, z_2) - |\gamma^{(1)}(z_1, z_2)|^2$$

Remark. The spectral decomposition of the one-particle density matrix indicates the statistical number of particles in the different one-particle states (also called **orbitals**). In particular, the eigenvalues 1 in (9.44) indicate that there is exactly 1 particle in each state f_j, which is certainly consistent with the Slater determinant. It should be emphasized, that it is only an intuition, and in the general case it can be misleading. The truth is that in a general N-body wave function ψ (or density matrix Γ) one cannot decouple the state individual particles. The typical chemistry picture, talking about different electrons occupying different one-particle orbital states, is fundamentally misleading: the two electrons of the Helium cannot be described as two independent electrons; they have complicated quantum correlation structure that is encoded in the corresponding two-body wave function $\psi(x_1, x_2)$ and cannot be described by one-particle wave functions. This fact does not, however, exclude the practical

usefulness of such orbital picture in certain regimes. Indeed various approximation theories (notably Hartree-Fock) rely on the orbital picture, and they give very good results.

The careful reader may notice a subtle point. Suppose Γ is a density matrix with spectral decomposition $\Gamma = \sum_j \mu_j |\Psi_j\rangle\langle\Psi_j|$. Let $\gamma^{(1)}$ be its one particle density matrix (one can do the same argument for any k, for simplicity we chose $k = 1$) and it also has a spectral decomposition $\gamma^{(1)} = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$ (note that capital letters denote N-particle wave functions). We would like to know the diagonal element of the kernel of $\gamma^{(1)}$. But as a kernel $\gamma^{(1)}(x, x')$ is defined only almost everywhere in (x, x'), so so setting $x = x'$ does not make sense a-priori. Of course we could say that we just *define*

$$\gamma^{(1)}(x, x) := \sum_j \lambda_j |\psi_j(x)|^2 \tag{9.45}$$

similarly as we *defined*

$$\Gamma(\mathbf{x}, \mathbf{x}) := \sum_j \mu_j |\Psi_j(\mathbf{x})|^2 \tag{9.46}$$

But now $\gamma^{(1)}(x, x)$ and $\Gamma(\mathbf{x}, \mathbf{x})$ should be related by

$$\gamma^{(1)}(x_1, x_1) = \int \Gamma(x_1, \widetilde{\mathbf{x}}; x_1, \widetilde{\mathbf{x}}) \mathrm{d}\widetilde{\mathbf{x}}$$

where $\widetilde{\mathbf{x}} = (x_2, \dots x_N)$. Are these definitions compatible? The answer is yes:

Theorem 9.4 *Let $\Gamma = \sum_j \mu_j |\Psi_j\rangle\langle\Psi_j|$ be an N-particle density matrix and $\gamma^{(1)} = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$ its one-particle marginal. Then*

$$\sum_j \lambda_j |\psi_j(x_1)|^2 = \sum_j \mu_j \int |\Psi_j(x_1, \widetilde{\mathbf{x}})|^2 \mathrm{d}\widetilde{\mathbf{x}} \tag{9.47}$$

for almost all x_1. In particular, for any function g of one variable, we have

$$Tr\Big[\sum_{j=1}^{N} g(x_j)\Big]\Gamma = Tr\, g\gamma^{(1)}$$

as long as at least one side is trace class. We recall that $\sum_j g(x_j)$ is the short-hand writing for the operator

$$g \otimes I \otimes \dots \otimes I + I \otimes g \otimes I \otimes \dots \otimes I + \dots + I \otimes \dots \otimes I \otimes g$$

Similar theorem holds for the k-particle marginals. In particular, for any function U of two variables we have

$$Tr\Big[\sum_{1\le i<j\le N} U(x_i - x_j)\Big]\Gamma = \frac{1}{2}\,TrU\gamma^{(2)}$$

as long as at least one side is trace class.

Proof. We will give only the proof of the first statement, the rest are analogous.

Let V be a bounded, real, measurable function on the one-particle space. Then, on one hand, by using the definition of $\gamma^{(1)}$ in terms of Ψ, we get

$$\langle\psi_i, V\gamma^{(1)}\psi_i\rangle = \sum_j \mu_j \int \overline{\psi_i(x)}\psi_i(x')V(x)\overline{\Psi_j(x, x_2, \dots x_N)}\Psi_j(x', x_2, \dots x_N)\mathrm{d}x\mathrm{d}x'\mathrm{d}x_2\mathrm{d}x_3\dots\mathrm{d}x_N,$$

and on the other hand, by using the spectral decomposition of $\gamma^{(1)}$ we get

$$\langle\psi_i, V\gamma^{(1)}\psi_i\rangle = \lambda_i \int V(x)|\psi_i(x)|^2\mathrm{d}x$$

We sum up these two identities for all i, to get

$$\int V(x)\sum_i \lambda_i|\psi_i(x)|^2\mathrm{d}x$$

$$= \sum_j \mu_j \int \left[\sum_i \int \overline{\psi_i(x)}\psi_i(x')V(x)\overline{\Psi_j(x, x_2, \dots x_N)}\Psi_j(x', x_2, \dots x_N)\mathrm{d}x\mathrm{d}x'\right]\mathrm{d}x_2\mathrm{d}x_3\dots\mathrm{d}x_N$$

For almost all $x_2, x_3, \dots x_N$, the function $x \to g(x) := \Psi_j(x, x_2, \dots x_N)$ is an L^2 function. Since V is bounded, so is the function $x \to V(x)\Psi_j(x, x_2, \dots x_N)$. Therefore in the square bracket we have

$$\Big[\dots\Big] = \sum_i \langle\bar{g}, \psi_i\rangle\langle\psi_i, V\bar{g}\rangle = \langle\bar{g}, V\bar{g}\rangle = \int V(x)|g(x)|^2$$

since ψ_i is an orthonormal basis. Thus we get

$$\int V(x)\sum_i \lambda_i|\psi_i(x)|^2\mathrm{d}x = \int V(x)\Big(\int \sum_j \mu_j|\Psi_j(x, x_2, \dots x_N)|^2\mathrm{d}x_2\mathrm{d}x_3\dots\mathrm{d}x_N\Big)\mathrm{d}x$$

Since this is true for any bounded V, we conclude that

$$\sum_i \lambda_i|\psi_i(x)|^2\mathrm{d}x = \int \sum_j \mu_j|\Psi_j(x, x_2, \dots x_N)|^2\mathrm{d}x_2\mathrm{d}x_3\dots\mathrm{d}x_N$$

and this was to be proven. The other statements can be proven similarly.

Alternatively, one can do an approximation/density argument. As long as Ψ_j and ψ_j are continuous, the statement is easy to show (test both sides with the characteristic function of a shrinking ball). The general case follows by using a smoothing (by convolution via an approximate delta function). $\square$

We have defined k-particle density matrices for all k, but actually only $k = 1, 2$ are important. The reason is that the energy of a typical interacting Hamiltonian with a two-body interaction can be expressed via one- and two-particle density matrices.

Let

$$H = \sum_{j=1}^{N} \big[-\Delta_j + V(x_j) \big] + \sum_{1 \le i < j \le N} U(x_i - x_j)$$

where U is a symmetric interaction potential. Let ψ a symmetric or antisymmetric N-particle wave function with marginals $\gamma^{(k)}$. Then, by symmetry,

$$\begin{aligned} \langle \psi, H\psi \rangle =& N \int \Big[|\nabla_{x_1} \psi(x_1, x_2, \dots x_N)|^2 + V(x_1) |\psi(x_1, x_2, \dots x_N)|^2 \Big] \mathrm{d}\mathbf{x} \\ &+ \frac{N(N-1)}{2} \int U(x_1 - x_2)) |\psi(x_1, x_2, \dots, x_N)|^2 \mathrm{d}\mathbf{x} \\ =& \operatorname{Tr} (-\Delta + V) \gamma^{(1)} + \frac{1}{2} \operatorname{Tr} U(x_1 - x_2) \gamma^{(2)} \end{aligned} \tag{9.48}$$

Now we see why the chosen normalization of the reduced density matrices is handy; all the explicit N factors are removed.

Note that $\operatorname{Tr} (-\Delta + V) \gamma^{(1)}$ is defined as before, i.e. we write up the spectral decomposition of $\gamma^{(1)} = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$ and

$$\operatorname{Tr} (-\Delta + V) \gamma^{(1)} = \sum_j \lambda_j \int |\nabla \psi_j|^2 + V |\psi_j|^2 \tag{9.49}$$

The potential part can be expressed by the one-particle density function,

$$\operatorname{Tr} V \gamma^{(1)} = \sum_j \lambda_j \int V |\psi_j|^2 = \int V \varrho$$

and similarly the two-body potential part is given by

$$\operatorname{Tr} U(x_1 - x_2) \gamma^{(2)} = \int U(x_1 - x_2) \gamma^{(2)}(x_1, x_2; x_1, x_2) \mathrm{d}x_1 \mathrm{d}x_2 = \int U(x - y) \varrho^{(2)}(x, y) \mathrm{d}x \mathrm{d}y$$

where, as in the one particle case, the two-particle density $\varrho^{(2)}$ is defined as the diagonal element of $\gamma^{(2)}$.

Remark. Formula (9.48) shows that the energy of an N-body system with a pair interaction potential in state ψ depends only on the two-particle density matrix $\gamma^{(2)}_\psi$ since the one-particle density matrix $\gamma^{(1)}$ can be expressed by $\gamma^{(2)}$: It is just the partial trace

$$\gamma^{(1)}(x,x') = \frac{1}{N-1}\int \gamma^{(2)}(x,y,x',y)\mathrm{d}y \tag{9.50}$$

Therefore, to find the ground state of an N-body system with pair interaction potential, it is actually sufficient to minimize (9.48) for all possible two-particle density matrices $\gamma^{(2)}$. In principle this should be much easier (especially numerically) than working with N-particle wave functions or density matrices. So one would hope that the true fermionic ground state energy

$$E_N := \inf\Big\{\langle\psi, H\psi\rangle, \|\psi\| = 1\Big\}$$

and the solution of the variational problem

$$\widetilde{E}_N := \inf\Big\{\mathrm{Tr}\,(-\Delta + V)\gamma^{(1)} + \frac{1}{2}\mathrm{Tr}\,U(x_1-x_2)\gamma^{(2)} \;:\; \mathrm{Tr}\,\gamma^{(2)} = N(N-1)\Big\}$$

(with the understanding that $\gamma^{(1)}$ is obtained via (9.50) from $\gamma^{(2)}$) are equal.

The problem is that not every two-body density matrix $\gamma^{(2)}$ (with the natural conditions, $\gamma^{(2)} \geq 0$, $\mathrm{Tr}\,\gamma^{(2)} = N(N-1)$) arises from some Γ with the required symmetry (either bosonic or fermionic). Unfortunately, there is no usable necessary and sufficient condition is known. This is called the **N-representability problem.**

Nevertheless, density matrix theories are very useful. Practically they often provide a good approximation. Theoretically they are important because they give a rigorous lower bound, from (9.48) it is clear that

$$E_N \geq \widetilde{E}_N$$

and recall that getting a *lower* bound for the true ground state energy E_N is typically much harder than getting an upper bound: the upper bound requires only a clever trial function ψ, while for a rigorous lower bound, in principle, one has to try out *all* wave functions. This can be replaced by trying to solve the minimization problem for $\widetilde{E}_N$; trying out "all" two-particle density matrices may be more feasible than trying out all N-body wave functions.

Again, the subtle reader may notice that when rewriting the kinetic energy of ψ into the kinetic energy of the one-particle density matrix in (9.48), we used a version of Theorem 9.4 for derivatives (and applied to a pure state instead of general Γ). The analogue of that theorem holds for the H^1 case as well, here we state only the result.

Theorem 9.5 *Let Γ be an N-particle H^1-density matrix, i.e.*

$$\Gamma = \sum_j \mu_j |\Psi_j\rangle\langle\Psi_j| \qquad with \quad \sum_j \mu_j \|\nabla\Psi_j\|^2 < \infty$$

Then its one particle marginal density $\gamma^{(1)}$ is also an H^1 density matrix, i.e. if $\gamma^{(1)} = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$ then $\sum_j \lambda_j \|\nabla\psi_j\|^2 < \infty$, moreover

$$\sum_j \mu_j \|\nabla\Psi_j\|^2 = \sum_j \lambda_j \|\nabla\psi_j\|^2 \tag{9.51}$$

Furthermore

$$\sum_j \mu_j \int |\nabla_{x_1}\Psi_j(x_1, \widetilde{\mathbf{x}})|^2 \mathrm{d}\widetilde{\mathbf{x}} = \sum_j \lambda_j |\nabla\psi(x_1)|^2 \tag{9.52}$$

for almost all x_1 and both sides are L^1 functions. This justifies that

$$Tr\Big[\sum_{j=1}^N (-\Delta_j)\Big]\Gamma = Tr(-\Delta)\gamma^{(1)} \tag{9.53}$$

where the corresponding traces are defined, in accordance with (9.45), (9.46), *as the two sides of* (9.51) *[note that the two traces are taken in two different spaces]. The more suggestive notation*

$$\sum_j Tr\nabla_j\Gamma\nabla_j = Tr\Big[\sum_{j=1}^N (-\Delta_j)\Big]\Gamma$$

is also used for the left hand side above, and similarly $Tr\nabla\gamma^{(1)}\nabla = Tr(-\Delta)\gamma^{(1)}$.

Moreover, the identity (9.52) *guarantees that for any function $g(x)$ of one variable we have*

$$\sum_j Tr\bar{g}(x_j)\nabla_j\Gamma\nabla_j g(x_j) = Tr\bar{g}\nabla\gamma^{(1)}\nabla g$$

and using (9.53) *for the density matrix $\sum_j g(x_j)\Gamma g(x_j)$ we have*

$$\sum_j Tr\nabla_j\bar{g}(x_j)\Gamma g(x_j)\nabla_j = Tr\nabla\bar{g}\gamma^{(1)}g\nabla$$

as long as one side is finite. In the second formula we can also use the notation

$$\sum_j Tr\nabla_j\bar{g}(x_j)\Gamma g(x_j)\nabla_j = Tr\Big[\sum_{j=1}^N g(x_j)(-\Delta_j)\bar{g}(x_j)\Big]\Gamma$$

and $Tr\nabla\bar{g}\gamma^{(1)}g\nabla = Trg(-\Delta)\bar{g}\gamma^{(1)}$.

10 Bosonic and fermionic density matrices

Let $\Psi(x_1, x_2, \dots x_N)$ be a normalized wave function and let $\gamma^{(1)} = \gamma^{(1)}_\Psi$ be its one-particle density matrix. We know that

$$\gamma^{(1)} \geq 0 \quad \text{and } Tr\gamma^{(1)} = N. \tag{10.54}$$

The same statement holds if we start with an N-particle density matrix Γ; its one-particle density matrix $\gamma^{(1)}$ also satisfies (10.54).

The converse also holds for bosonic density matrices:

Theorem 10.1 *Let the bounded self-adjoint operator γ on $L^2(\mathbf{R}^d)$ satisfy $\gamma \geq 0$ and $Tr\gamma = N$. Then there is a bosonic N-particle density matrix Γ such that its one-particle marginal, $\gamma^{(1)}$ coincides with γ. Moreover, if $N \geq 2$, then Γ can be chosen to be a pure state. Thus one-particle density matrices satisfying $\gamma \geq 0$ and $Tr\gamma = N$ are called* **admissible one-particle density matrices for bosons.**

Proof. For $N = 1$ just take $\Gamma = \gamma$. For $N \geq 2$, consider the spectral decomposition $\gamma = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|$ with orthonormal functions ϕ_i and $\lambda_i > 0$. Now we can build the normalized wave function

$$\Psi(\mathbf{x}) = N^{-1/2} \sum_i \lambda_i^{1/2} \phi_i(x_1)\phi_i(x_2) \dots \phi_i(x_N)$$

and it is easy to CHECK [!!] (using the orthogonality of ϕ_i's) that $\gamma^{(1)}_\Psi = \gamma$. □

Thus we could characterize one-particle density matrices for bosons via their natural properties (10.54). However, if Ψ is a fermionic wave function, then there is a further restriction on $\gamma^{(1)}$:

Theorem 10.2 *Let $\gamma^{(1)}$ be the one-particle density matrix of a normalized antisymmetric function Ψ. Then*

$$\gamma^{(1)} \leq I \tag{10.55}$$

i.e. all eigenvalues of $\gamma^{(1)}$ are at most 1. The same statement holds for the one particle density matrix of an arbitrary fermionic density matrix Γ. The converse of the statement also holds: if $0 \leq \gamma^{(1)} \leq 1$, with $Tr\gamma^{(1)} = N$, then there exists an N-particle fermionic density matrix Γ such that $\gamma^{(1)}$ is its one-particle marginal. In general, Γ is not a pure state. Therefore, density matrices $\gamma^{(1)}$ satisfying $0 \leq \gamma^{(1)} \leq I$ are called **admissible one-body density matrices for fermions**.

Remark. As it was mentioned in Exercise 9.3, the spectral decomposition

$$\gamma^{(1)} = \sum_j \lambda_j |\phi_j\rangle\langle\phi_j| \tag{10.56}$$

indicates that the distribution of the one-particle orbitals in the state Ψ: intuitively it says that the "number" of particles in state ϕ_j is λ_j. If we combine this intuition with the Pauli principle, then it is immediately clear that the fermionic nature implies $\lambda_j \leq 1$ for all j. This sounds like an almost honest proof of the above theorem, but it heavily relies on the orbital picture.

Proof of Theorem 10.2. To show that $\gamma^{(1)} \leq 1$, we have to prove that

$$\langle f, \gamma^{(1)} f\rangle \leq \|f\|_2^2 \tag{10.57}$$

for any $f \in L^2(\mathbf{R}^d)$. Define

$$K(x_1, x_2, \ldots x_N, y_1, \ldots y_N) := \sum_{j=1}^N f(x_j)\bar{f}(y_j)$$

which is just a kernel of an operator that is the sum of rank-one projections. With fancy notation

$$K = |f\rangle\langle f| \otimes I \otimes \ldots \otimes I + I \otimes |f\rangle\langle f| \otimes I \otimes \ldots \otimes I + \ldots + I \otimes \ldots \otimes I \otimes |f\rangle\langle f|$$

Let $f = f_0, f_1, f_2, \ldots$ be an orthonormal basis (i.e. extend f to an ONB). By Exercise 3.1 the functions

$$f_{\wedge J} = f_{j_1} \wedge f_{j_2} \wedge \ldots \wedge f_{j_N}$$

for $J = (j_1, j_2, \ldots, j_N) \in \mathbf{N}^N$ with distrinct elements ($j_\ell \neq j_k$ for $j \neq k$) form a basis in the space of antisymmetric functions. This basis is an eigenbasis of K since, clearly,

$$K f_{\wedge J} = E(J) f_{\wedge J}$$

where $E(J) = 1$ if $j_\ell = 0$ for some ℓ, and $E(J) = 0$ otherwise. Thus

$$\langle f_{\wedge J}, K f_{\wedge J}\rangle \leq 1 \tag{10.58}$$

We now write Ψ in this basis:

$$\Psi = \sum_J C(J) f_{\wedge J} \tag{10.59}$$

where the summation runs over all index sets J's with distinct indices. Since $f_{\wedge J}$ is antisymmetric under any permutation of the indices in J, the function

$$C(J) = C(j_1, j_2, \dots j_N)$$

must also be antisymmetric, in particular, C vanishes if any two indices coincide (or, in other words, the summation is restriced to all J's with distinct elements). By normalization

$$\sum_J |C(J)|^2 = 1$$

Using (10.59) and (10.58), we compute

$$\langle \Psi, K\Psi \rangle = \sum_J |C(J)|^2 \langle f_{\wedge J}, K f_{\wedge J} \rangle \leq 1$$

But

$$\langle \Psi, K\Psi \rangle = \sum_{i=1}^{N} \int \bar{\Psi}(x_1, \dots, x_i, \dots x_N) f(x_i) \bar{f}(x_i') \Psi(x_1, \dots, x_i', \dots x_N) \mathrm{d}x_1 \dots \mathrm{d}\widehat{x_i} \dots \mathrm{d}x_N$$

$$= \langle f, \gamma_\Psi^{(1)} f \rangle$$

which proves (10.55) for the case of fermionic wavefunctions.

Finally, the proof for an arbitrary fermionic density matrix is straighforward from the spectral decomposition

$$\Gamma = \sum_k \mu_k |\Psi_k\rangle\langle\Psi_k|$$

since here each Ψ_k is a fermionic wave function with one particle density matrix $\gamma_k^{(1)}$. Thus the one-particle density matrix of Γ is given by

$$\gamma^{(1)} = \sum_k \mu_k \gamma_k^{(1)}$$

Since $\sum_k \mu_k = 1$ and μ_k's are positive, from $\gamma_k^{(1)} \leq 1$ it immediately follows that $\gamma^{(1)} \leq 1$.

We will now sketch the proof of the converse. Consider the spectral decomposition (10.56) of $\gamma^{(1)}$, order the eigenvalues decreasingly, $1 \geq \lambda_1 \geq \lambda_2 \leq$ and we have $\sum_j \lambda_j = N$.

The claim is that there exists countable many subsets $S_1, S_2, \ldots$ of the index set $\{1, 2, \ldots\}$, each with N elements, $|S_j| = N$, such that

$$\lambda_j = \sum_{k=1}^{K} c_k \mathbf{1}_{S_j}(k) \tag{10.60}$$

with some appropriate positive constants c_k with $\sum_k c_k = 1$ (here $\mathbf{1}_S$ is the characteristic function of the set S). The summation is either finite or infinite, i.e. $K \leq \infty$.

To see this, we note that if $\lambda_1 = \lambda_2 = \ldots \lambda_N = 1$, then we just choose $K = 1$, $c_1 = 1$ and $S_1 = \{1, 2, 3, \ldots, N\}$.

Otherwise, set $\varepsilon = \min\{\lambda_N, 1 - \lambda_{N+1}\}$, which now satisfies $\varepsilon > 0$, and write

$$\lambda_j = \varepsilon \mathbf{1}_{[1,N]}(j) + (1 - \varepsilon) f_j$$

with

$$f_j = \frac{1}{1 - \varepsilon} \Big(\lambda_j - \varepsilon \mathbf{1}_{[1,N]}(j) \Big) \tag{10.61}$$

It is easy to check that $0 \leq f_j \leq 1$ and $\sum_j f_j = N$, i.e. the sequence f_j satisfies the same conditions as λ_j.

After rearranging the sequence f_j in decreasing order, we repeat the same construction for the f's and one gets

$$\lambda_j = \varepsilon \mathbf{1}_{[1,N]}(j) + (1 - \varepsilon)\varepsilon' \mathbf{1}_S(j) + (1 - \varepsilon)(1 - \varepsilon') g_j$$

where S is the index set of the N biggest f's and g_j is defined analogously to (10.61). One can iterate this procedure and it is not very hard to see (but will not proven here), that the remainders, having the prefactors $(1 - \varepsilon)(1 - \varepsilon')(1 - \varepsilon'') \ldots$, eventually vanish. This proves the representation (10.60).

Once (10.60) is given, we can simply construct a density matrix that is a convex linear combination of rank-one projections onto Slater determinants:

$$\Gamma = \sum_{k=1}^{K} c_k \Gamma_{\Psi_k}, \quad \Psi_k = f_{j_1} \wedge f_{j_2} \wedge \ldots \wedge f_{j_N} \text{ with } S_k = \{j_1, j_2, \ldots, j_N\}$$

It is easy to CHECK [!!] that the one particle marginal density matrix of Γ is $\gamma^{(1)}$. $\square$

11 Creation and annihilation operators

There is a simple formalism to shorten the proof of (10.57) for the marginal density of N-particle wave functions Ψ. For any $\phi \in \mathcal{H} = L^2(\mathbf{R}^d)$ we define the **annihilation operator** $a_{N,\phi} : \mathcal{H}_N := \bigwedge_1^N \mathcal{H} \mapsto \mathcal{H}_{N-1} := \bigwedge_1^{N-1} \mathcal{H}$ as follows

$$(a_{N,\phi}\Psi)(x_1, \dots x_{N-1}) = N^{1/2} \int \Psi(x_1, \dots x_{N-1}, x_N)\bar{\phi}(x_N)\mathrm{d}x_N$$

We also define the **creation operator** $a^\dagger_{N,\phi} : \bigwedge_1^{N-1} \mathcal{H} \mapsto \bigwedge_1^N \mathcal{H}$ as

$$(a^\dagger_{N,\phi}\Phi)(x_1, \dots x_{N-1}, x_N) = N^{-1/2}\mathcal{A}\big[\Phi(x_1, \dots x_{N-1})\phi(x_N)\big]$$

A simple calculation shows that they are adjoints of each other in the following sense:

$$\langle \Phi, a_{N,\phi}\Psi\rangle_{\mathcal{H}_{N-1}} = \langle a^\dagger_{N,\phi}\Phi, \Psi\rangle_{\mathcal{H}_N} \tag{11.62}$$

for any $\Phi \in \mathcal{H}_{N-1}$ and $\Psi \in \mathcal{H}_N$. Moreover, they satisfy the following **anticommutation relation**:

$$a_{N+1,\phi}a^\dagger_{N+1,\phi} + a^\dagger_{N,\phi}a_{N,\phi} = \|\phi\|^2 I_N \tag{11.63}$$

(where I_N is the identity on $\mathcal{H}_N$).

Exercise 11.1 (IMPORTANT) *Verify* (11.62) *and* (11.63)

So far we described a Hilbert space of states with a fixed particle number N. The following construction gives the framework to describe states with variable particle numbers. We define the **fermionic Fock space** (in algebraic sense):

$$\mathcal{F}(\mathcal{H}) := \bigoplus_{N=0}^{\infty} \bigwedge_1^N \mathcal{H} \tag{11.64}$$

where, by convention, $\bigwedge_1^0 \mathcal{H} = \mathbf{C}$. The elements of the fermionic Fock space are sequences of antisymmetric functions with increasing number of variables:

$$F \in \mathcal{F}(\mathcal{H}) \mapsto (F_0, F_1, F_2, \dots), \qquad F_0 \in \mathbf{C},\ F_N \in \bigwedge_1^N \mathcal{H}, \quad (N \geq 1)$$

The Fock space is equipped with a natural scalar product

$$\langle F, G\rangle_{\mathcal{F}(\mathcal{H})} := \sum_{N=0}^{\infty} \langle F_N, G_N\rangle_{\mathcal{H}_N}$$

To do analysis, one restricts the attention to elements with finite norm, i.e. in mathematical physics usually one considers

$$\mathcal{F}(\mathcal{H}) = \Big\{ F \in \bigoplus_{N=0}^{\infty} \bigwedge_{1}^{N} \mathcal{H} \ : \ \langle F, F \rangle = \sum_{N=0}^{\infty} \|F_N\|^2_{\mathcal{H}_N} < \infty \Big\} \tag{11.65}$$

The interpretation is that an element of the Fock space describes a state with variable particle number; $F_N(x_1, \dots x_N)$ being the wave function describing the state in the N**-particle sector**. For a normalized element of the Fock space, $\|F\|_{\mathcal{F}} = 1$, we have

$$1 = \|F\|^2_{\mathcal{F}} = \sum_{N=0}^{\infty} \|F_N\|^2_{\mathcal{H}_N}$$

and the quantity $\|F_N\|^2_{\mathcal{H}_N}$ expresses the probability that there are exactly N particles.

The natural basis element in the zero-particle sector is called **vacuum**, and is traditionally denoted by $\Omega \in \mathcal{F}(\mathcal{H})$:

$$\Omega = (1, 0, 0, \dots)$$

The vacuum state expresses the fact that with probability one there is no particle around. It is important to emphasize, that **the vacuum is not the zero vector**. The vacuum is an honest quantum state, thus it is described by a normalized element of the Fock space.

Moroever, it is important to distinguish between the Fock space as an algebraic object (11.64) and as a Hilbert space. Rigorous analysis can only be done in (11.64).

The creation and annihilation operators naturally extend to the whole Fock space, we simply define $a^\dagger_\phi$ and a_ϕ just by their restrictions on the N-particle sector:

$$a_\phi,\, a^\dagger_\phi : \ \mathcal{F}(\mathcal{H}) \mapsto \mathcal{F}(\mathcal{H})$$

$$a_\phi\Big|_{\mathcal{H}_N} := a_{N,\phi}, \qquad a^\dagger_\phi\Big|_{\mathcal{H}_{N-1}} := a^\dagger_{N,\phi}$$

Note, in particular, that the following extensions of (11.62) and (11.63) hold on $\mathcal{F}(\mathcal{H})$:

$$\langle F, a^\dagger_\phi G \rangle = \langle a_\phi F, G \rangle, \qquad F, G \in \mathcal{F}(\mathcal{H})$$

and

$$a_\phi a^\dagger_\phi + a^\dagger_\phi a_\phi = \|\phi\|^2 I, \qquad \text{or, in more general} \qquad a_\phi a^\dagger_\psi + a^\dagger_\phi a_\psi = \langle \phi, \psi \rangle I \tag{11.66}$$

where I denotes the identity on $\mathcal{F}(\mathcal{H})$. This last relation is called the **canonical anticommutation relation (CAR)**.

Exercise 11.2 *Let $\{\phi_0, \phi_1, \ldots\} \subset \mathcal{H}$ be an orthonormal basis in $\mathcal{H}$. Show that*

$$\mathcal{F}(\mathcal{H}) = \overline{Span\Big\{ \prod_{j\in K} a^\dagger_{\phi_j}\Omega \ : \ K \subset \mathbf{N}, |K| < \infty \Big\}}$$

where K runs through all finite subsets of the index set $\mathbf{N}$.

Hint: Show that the creation operators "create" Slater determinants out of the vacuum, e.g.

$$a^\dagger_\phi \Omega = (0, \phi, 0, 0, \ldots)$$

$$a^\dagger_\phi a^\dagger_\psi \Omega = (0, 0, \phi \wedge \psi, 0, 0, \ldots)$$

if $\phi \perp \psi$, etc. (and similarly the annihilation operators, acting on appropriate Slater determinants, eliminate a factor).

Exercise 11.3 *Think over the necessary modifications for the bosonic case (i.e. define the bosonic Fock space, the corresponding creation and annihilation operators) and derive the canonical commutation relations*

$$a_\phi a^\dagger_\phi - a^\dagger_\phi a_\phi = \|\phi\|^2 I, \qquad \text{or, in more general} \qquad a_\phi a^\dagger_\psi - a^\dagger_\phi a_\psi = \langle \phi, \psi \rangle I \tag{11.67}$$

*for the appropriately defined bosonic operators (***canonical commutation relations***).*

Exercise 11.4 *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces. Prove that*

$$\mathcal{F}(\mathcal{H}_1 \oplus \mathcal{H}_2) = \mathcal{F}(\mathcal{H}_1) \otimes \mathcal{F}(\mathcal{H}_2)$$

holds for both the fermionic and bosonic Fock space (in the sense that there is a natural isometry).

After all these prerequisites, we can give a short alternative proof of (10.57) if $\Psi \in \mathcal{H}_N$, $\|\Psi\| = 1$. Using the identity (11.68) and the anticommutation relation (11.63), we simply compute

$$\begin{aligned} \langle \phi, \gamma^{(1)} \phi \rangle &= \langle \Psi, a^\dagger_{N,\phi} a_{N,\phi} \Psi \rangle = \langle \phi, \phi \rangle \langle \Psi, \Psi \rangle_{\mathcal{H}_N} - \langle \Psi, a_{N+1,\phi} a^\dagger_{N+1,\phi} \Psi \rangle \\ &= \langle \phi, \phi \rangle - \langle a^\dagger_{N+1,\phi} \Psi, a^\dagger_{N+1,\phi} \Psi \rangle \leq \langle \phi, \phi \rangle \qquad \square \end{aligned}$$

A very important fact: A-priori it is unclear whether a_ϕ and $a^\dagger_\phi$ can indeed be extended to act on any element of $\mathcal{F}(\mathcal{H})$. The operators $a_{N,\phi}$ and $a^\dagger_{N,\phi}$ are bounded, but if one naively estimates their norm, the bound is $N^{1/2}$:

$$\|a_{N,\phi}\Psi\|^2_{\mathcal{H}_{N-1}} = \langle a_{N,\phi}\Psi, a_{N,\phi}\Psi \rangle_{\mathcal{H}_{N-1}} = \langle \phi, \gamma^{(1)} \phi \rangle \tag{11.68}$$

and since $\operatorname{Tr}\gamma^{(1)} = N$, a-priori we only know that $\|\gamma^{(1)}\| \leq N$, thus

$$\|a_{N,\phi}\| \leq N^{1/2}\|\phi\|$$

and it is easy to see that similarly

$$\|a^\dagger_{N,\phi}\| \leq N^{1/2}\|\phi\|$$

However, by (11.66) and by the fact that both $a_\phi a^\dagger_\phi$ and $a^\dagger_\phi a_\phi$ are (formally) nonnegative operators, it follows that

$$\|a_{N,\phi}\| \leq \|\phi\|, \qquad \|a^\dagger_{N,\phi}\| \leq \|\phi\|$$

and it is very easy to see that actually there is equality.

The precise proof is elementary: one first defines a_ϕ and $a^\dagger_\phi$ on the subspace of $\mathcal{F}(\mathcal{H})$ that contains only finite number of nonzero F_N coordinates; this subspace is dense and the operators a_ϕ and $a^\dagger_\phi$ are bounded, so by the bounded extension principle (see, e.g. Reed-Simon Vol I. Thm I.7) they can be extended as bounded operators onto the whole $\mathcal{F}(\mathcal{H})$.

12 Ground state of non-interacting fermions

Theorem 12.1 *Let V satisfy the usual conditions, i.e $V \in L^{d/2} + L^\infty$ and V vanishes at infinity. Then we know that the ground state energy of $h = -\Delta + V$ is not $-\infty$ and suppose that there are at least N negative eigenvalues, $e_0 \leq e_1 \leq \ldots \leq e_{N-1} < 0$, with orthonormal eigenfunctions $f_0, f_1, \ldots$. Then the ground state energy of N non-interacting fermions* (4.9) *(with $W \equiv 0$) is given by the sum of the N lowest (negative) eigenvalues*

$$E^f_0(N) = \sum_{i=0}^{N-1} e_i$$

and the corresponding minimizer is given by the Slater determinant of the one-particle eigenfunctions

$$\psi_0 = \bigwedge_{i=0}^{N-1} f_i$$

If the number of negative eigenvalues is less than N, then the ground state energy is given by the sum of all negative eigenvalues

$$E^f_0(N) = \sum_{i\,:\,e_i<0} e_i$$

and there is no minimizer in the problem (4.9).

As it will be clear from the proof, the fermionic ground state is unique only if $e_0, e_1, \dots e_{N-1}$ are all non-degenerate. In case of degeneracy, one has a choice to select different eigenbases in that eigenspace and build different Slater determinants on them. However, by Exercise 3.1 part iii) indicates that the **many body density** function, $|\psi(\mathbf{x})|^2$, is unique, if all degenerate shells are completely filled.

You may notice that we tacitly assumed that the number of spin states $q = 1$, which, strictly speaking, is wrong for fermions (q has to be even). As long as h is spin-independent, the same argument gives the following result:

$$E_0^f(N) = q \sum_{i=0}^{[\frac{N}{q}]-1} e_i + \Big(N - q[\frac{N}{q}]\Big) e_{[\frac{N}{q}]+1}$$

where $[\cdot]$ denotes the integer part. The formula is complicated, but it just expresses the fact that one fills up all low lying levels with a maximum multiplicity q (and the last level is only partially filled).

Theorem 12.1 deals with a fixed number of particles. In some situations we may think of the number particles not fixed, e.g. we may not know a-priori, how many electrons can be bound to a nucleus. In this case, the number of electrons N can also be subject to a variational principle. The interpretation is that if a system energetically favors one more electron, it can always find one in the "infinite" electron reservoir of the world, or, in contrary, if it would be energetically favorable to have one less electron, the system can always "dump" the extra electron out to an infinite distance.

The following corollary is expresses this situation and its proof is obvious:

Corollary 12.2 *If the number of particles is not fixed, then the absolute ground state energy of the non-interacting fermionic system is given by the sum of all negative eigenvalues*

$$\inf_N E_0^f(N) = \sum_{i\,:\,e_i<0} e_i$$

(with the understanding that it may be $-\infty$).

Remark. Similarly to the remark after Theorem 5.1, the above theorem for fermions holds for general operators of the form $\sum_i h_i$, where h is a one-particle operator whose quadratic form is bounded from below.

In the special case, when h has a complete set of eigenvectors $v_0, v_1, \ldots$ with eigenvalues $e_0 \leq e_1 \leq \ldots$, we can prove Theorem 12.1 directly. We recall from Exercise (3.1) that the tensor-product space $\bigwedge_{i=1}^N \mathcal{H}$ has a natural orthonormal basis of the form

$$\{\mathbf{v}_{\wedge J} \ : \ J = (j_1, j_2, \ldots, j_N) \in \mathbf{N}^N, j_\ell \neq j_k\}$$

where for any $J = (j_1, j_2, \ldots, j_N) \in \mathbf{N}^N$ with distinct components we define

$$\mathbf{v}_{\wedge J} = v_{j_1} \wedge v_{j_2} \wedge \ldots \wedge v_{j_N}$$

It is easy to see that

$$\Big(\sum_{i=1}^N h_i\Big)\mathbf{v}_{\wedge J} = \Big(\sum_{i=1}^N e_{j_i}\Big)\mathbf{v}_{\wedge J}$$

thus the set

$$\{\mathbf{v}_{\wedge J} \ : \ J \in \mathbf{N}^N, J \text{ has distinct components}\}$$

forms a complete eigenbasis for $\sum_i h_i$. The lowest eigenvalue is of course

$$\min_{J \,:\, j_\ell \neq j_k} \sum_{i=1}^N e_{j_i} = e_0 + e_1 + \ldots + e_{N-1}$$

The corresponding eigenfunction has the property that the lowest energy one-particle states are occupied. In physics terminology, **the energy levels are filled up from below.**

Proof of Theorem 12.1. Let Ψ be an arbitrary normalized fermionic wave function with density matrix $\gamma^{(1)}$ and

$$\gamma^{(1)} = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$$

be its spectral decomposition. From Theorem 10.2 we know that $\lambda_j \leq 1$. The energy of Ψ is given by

$$\mathcal{E}(\Psi) = \sum_j \lambda_j \int \left[|\nabla\psi_j|^2 + V|\psi_j|^2\right]$$

from (9.48) and (9.49). Now we can write

$$\psi_j = \sum_\ell c_{j\ell} f_\ell + q_j \tag{12.69}$$

where $f_0, f_1, \ldots$ are the eigenfunctions of h and q_j is an element in the orthogonal complement of the span of these eigenfunctions. Note that $q_j \in H^1$ since $\psi_j \in H^1$ and all $f_\ell \in H^1$. From the normalization

$$\|q_j\|^2 + \sum_\ell |c_{j\ell}|^2 = 1$$

we get

$$\sum_\ell |c_{j\ell}|^2 \leq 1 \tag{12.70}$$

We know that

$$\int |\nabla q_j|^2 + V|q_j|^2 \geq 0$$

(following from the fact that q_j is orthogonal to all states that have negative energy) and

$$\int \nabla \bar{f_\ell} \cdot \nabla f_k + V \bar{f_\ell} f_k = e_k \delta_{k=\ell}$$

(following from the construction of excited states) and

$$\int \nabla \bar{f_\ell} \cdot \nabla q_j + V \bar{f_\ell} q_j = 0$$

(following from the weak solution $(-\Delta + V) f_\ell = e_\ell f_\ell$ after testing against $q_j \in H^1$ and using $q_j \perp f_\ell$).

Using these formulas and (12.69), we can estimate

$$\int \left[|\nabla \psi_j|^2 + V|\psi_j|^2 \right] \geq \sum_\ell |c_{j\ell}|^2 e_\ell$$

Thus

$$\mathcal{E}(\psi) \geq \sum_j \lambda_j \sum_\ell |c_{j\ell}|^2 e_\ell = \sum_\ell \mu_\ell e_\ell$$

with $\mu_\ell = \sum_j \lambda_j |c_{j\ell}|^2$. Using $\lambda_j \leq 1$, $\sum_j \lambda_j = N$ and the fact that $\{\psi_j\}$ and $\{f_\ell\}$ are both orthonormal systems, we have

$$\mu_\ell \leq \sum_j |c_{j\ell}|^2 = \sum_j |\langle f_\ell, \psi_j \rangle|^2 \leq \|f_\ell\|^2 \leq 1$$

and

$$\sum_\ell \mu_\ell = \sum_j \lambda_j \sum_\ell |c_{j\ell}|^2 \leq \sum_j \lambda_j = N$$

(in the last step we used (12.70)).

Thus we proved that

$$\mathcal{E}(\psi) \geq \inf\{\sum_\ell \mu_\ell e_\ell \ : \ 0 \leq \mu_\ell \leq 1, \ \sum_\ell \mu_\ell \leq N\}$$

where $e_0 \leq e_1 \leq \ldots \leq 0$. Now we solve the minimization problem on the right hand side. Clearly we get the smallest value, if we select the maximum allowed weight $\mu_0 = 1$ assigned to the smallest number e_0, then the next maximal weight $\mu_1 = 1$ to the next smallest number etc. Therefore, the solution of the above problem is $\sum_{\ell=0}^{N-1} e_\ell$ if there are at least N negative eigenvalues and $\sum_{e_\ell<0} e_\ell$ (summation of all negative values) if there are less than N negative eigenvalues.

Taking the infimum over all ψ, we proved that

$$E_0^f(N) \geq \sum_{i=0}^{N-1} e_i$$

in the first case or

$$E_0^f(N) \geq \sum_{e_i<0} e_i$$

in the second case.

The opposite inequality can be easily obtained by a trial state consisting of the Slater determinant of the first N eigenfunctions in the first case. In the second case we take the Slater determinant of all eigenfunctions with negative eigenvalues plus a few other functions that are orthogonal, located far out in infinity and have very small kinetic energy (very flat). A small calculation shows that with such function the lower bound $\sum_{e_i<0} e_i$ on the energy can be arbitrarily approximated. This completes the proof. □

13 Min-max principle

Suppose we have two potentials, $V(x)$ and $W(x)$, such that $V(x) \leq W(x)$. We would like to compare the energy levels $E_0 \leq E_1 \leq E_2 \leq \ldots$ of $-\Delta + V$ with those of $-\Delta + W$, denoted by $E_0' \leq E_1' \leq E_2' \leq \ldots$. From the variational principle for the ground state

$$E_0 = \inf\Big\{ \int |\nabla\psi|^2 + V|\psi|^2 \ : \ \psi \in H^1, \|\psi\| = 1\Big\}$$

it is obvious that $E_0 \leq E_0'$. The following theorem shows that the same is true for all eigenvalues, i.e.

$$E_j \leq E_j' \tag{13.71}$$

in particular we obtain a comparison for the bosonic and fermionic ground states for N non-interacting particles subject to the potential V and W.

This theorem is known under the name of "Min-Max" principle and it has several versions.

Theorem 13.1 *Let $V \in L^{d/2} + L^\infty$ in $d \geq 3$ dimensions (and similar conditions in $d = 1, 2$ dimensions) and assume that V vanishes at infinity. Let $\phi_0, \phi_1, \dots \phi_{k-1}$ be any k orthonormal functions and assume that $\phi_j \in H^1$.*

(i) Construct the $k \times k$ hermitian matrix $\widehat{h}$ with entries

$$(\widehat{h})_{ij} := h_{ij} = \int \nabla \bar{\phi}_i \cdot \nabla \phi_j + \int V \bar{\phi}_i \phi_j$$

Let $\lambda_0 \leq \lambda_1 \leq \ldots \leq \lambda_{k-1}$ be the eigenvalues of $\widehat{h}$, ordered increasingly. Then

$$E_j \leq \lambda_j \qquad j = 0, 1, \dots, k-1$$

(ii) [Max-Min] Suppose that for some $k \geq 0$, E_k is still an eigenvalue. Then

$$E_k = \max_{\phi_0, \dots \phi_{k-1}} \min \left\{ \mathcal{E}(\phi_k) \ : \ \phi_k \perp \phi_0, \dots \phi_{k-1} \right\} \tag{13.72}$$

where the maximum is taken for all collections of k functions (not necessarily orthonormal, although without loss of generality one may restrict the minimization only for orthonormal collections).

(iii) [Min-Max] Suppose that for some $k \geq 0$, E_k is still an eigenvalue. Then

$$E_k = \min_{\phi_0, \dots \phi_k} \max \left\{ \mathcal{E}(\phi) \ : \ \phi \in \mathit{Span}(\phi_0, \dots \phi_k) \right\} \tag{13.73}$$

Here the minimum is taken over all collections of k linearly independent functions (not necessarily orthonormal, but without loss of generality one may restrict the minimization only for orthonormal collections).

If E_k is not an eigenvalue, then min *becomes* inf *in both formulas* (13.72) *and* (13.73)

Parts (i) and (iii) give upper bounds for the true eigenvalues. Part (i) is computationally more feasible since it reduces the question to computing eigenvalues of a finite matrix. Part (ii) can in principle give lower bounds for the eigenvalues, but in general the minimization problem within the formula is as hard as the original problem.

The inequality (13.71) follows immediately from both the Min-max and Max-min principles, using the fact that $\mathcal{E}(\phi) \leq \mathcal{E}'(\phi)$, where $\mathcal{E}$ and $\mathcal{E}'$ are the quadratic forms of $-\Delta + V$ and $-\Delta + W$.

Proof. Part (i): Let $\mathbf{v}_j$, $j = 0, 1, \ldots, k-1$ be orthonormal eigenvectors of $\widehat{h}$. Set $\chi_j = \sum_{i=0}^{k-1} \mathbf{v}_j(i)\phi_i$, then

$$\|\chi_j\|^2 = \sum_{i=0}^{k-1} |\mathbf{v}_j(i)|^2 = 1$$

and

$$E_0 \le \int |\nabla \chi_0|^2 + \int V|\chi_0|^2 = \sum_{i,i'} \bar{\mathbf{v}}_0(i)\mathbf{v}_0(i')h_{ii'} = \lambda_0$$

Now we show the inequality for a general $m \le k-1$. Since $\chi_0, \chi_1, \ldots \chi_m$ are orthonormal, they form an $(m+1)$-dimensional space. Let $\psi_0, \psi_1, \ldots \psi_{m-1}$ be the eigenfunctions of $-\Delta + V$, they form an m-dimensional space, therefore there is a normalized function

$$\chi = \sum_{j=0}^{m} c_j \chi_j$$

such that $\chi \perp \psi_\ell$, $\ell = 0, 1, 2 \ldots m-1$. Thus χ can be used as a trial function in the definition of E_m:

$$E_m \le \mathcal{E}(\chi) = \int |\nabla \chi|^2 + \int V|\chi|^2 = \sum_{j,j'=0}^{m} \sum_{i,i'=0}^{k-1} \overline{c_j \mathbf{v}_j(i)} c_{j'} \mathbf{v}_{j'}(i') h_{ii'} = \sum_{j=0}^{m} |c_j|^2 \lambda_j \qquad (13.74)$$

using that

$$\sum_{i,i'=0}^{k-1} \bar{\mathbf{v}}_j(i) h_{ii'} \mathbf{v}_{j'}(i') = \lambda_j \delta_{jj'}$$

But then clearly

$$\sum_{j=0}^{m} |c_j|^2 \lambda_j \le \lambda_m \sum_{j=0}^{m} |c_j|^2 = \lambda_m$$

which proves that $E_m \le \lambda_m$.

In the argument above we tacitly assumed that $E_{k-1} < 0$, i.e. the eigenfunctions $\psi_0, \psi_1, \ldots \psi_{k-1}$ indeed exist. If fewer of them exist (i.e. if the number of negative eigenvalues n is smaller than k), then we can still complete the proof: the above argument shows that $E_j \le \lambda_j$, for $j \le n-1$, so we just need to show that $\lambda_n \ge 0$ (since $E_n = E_{n+1} = \ldots = 0$). Suppose $\lambda_n < 0$. From (13.74) it is clear that

$$\mathcal{E}(\chi) \le \lambda_n < 0$$

for any normalized χ of the form $\chi = \sum_{j=0}^{n} c_j \chi_j$. We can find a χ of this form that is orthogonal to $\psi_0, \psi_1, \ldots \psi_{n-1}$, thus we would violate the definition of E_n:

$$0 = E_n = \inf \left\{ \mathcal{E}(\psi) \ : \ \|\psi\| = 1, \psi \perp \psi_j, \ 0 \leq j \leq n-1 \right\}$$

This completes the proof.

Part (ii): Let

$$\gamma_k := \max_{\phi_0, \ldots \phi_{k-1}} \min \left\{ \mathcal{E}(\phi_k) \ : \ \phi_k \perp \phi_0, \ldots \phi_{k-1} \right\}$$

and let $\psi_0, \ldots \psi_{k-1}$ be the eigenfunctions belonging to $E_0, \ldots E_{k-1}$. By definition of E_k, we have

$$E_k = \min \left\{ \mathcal{E}(\phi) \ : \ \phi \perp \psi_0, \ldots \psi_{k-1} \right\}$$

and thus clearly

$$E_k \leq \gamma_k$$

On the other hand, for any choice of $\phi_0, \ldots \phi_{k-1}$ there is always a linear combination $f = \sum_{j=0}^{k} c_j \psi_j$ that is orthogonal to each of ϕ_i, $0 \leq i \leq k-1$ (CHECK! the main reason is that the former spans a k-dimensional space, the latter linear combinations span a $(k+1)$-dimensional space). But

$$\mathcal{E}(f) = \sum_{j=0}^{k} |c_j|^2 E_j \leq E_k$$

thus

$$\min\{ \mathcal{E}(f) \ : \ f \perp \phi_0, \ldots, \phi_{k-1} \} \leq E_k$$

so after taking the maximum over all ϕ_i's, we get $\gamma_k \leq E_k$

The proof of Part (iii) is very similar to that of Part (ii) and left as an exercise (CHECK!) $\square$