Free Quantum Gases

Let us analyse the KMS-states for the free quantum gases starting with Fermions.

Remember, we start from a 1-particle Hilbert space $\mathfrak{h}$ and obtain creation and annihilation operators $a(f)$, $a^*(g)$ for $f,g \in \mathfrak{h}$.

$$\{a(f), a^*(g)\} = \langle f, g \rangle.$$

The time evolution is given by a Hamiltonian $H : \mathfrak{h} \to \mathfrak{h}$ in the 1-particle HS via (typically unbounded)

$$\alpha_t(a(f)) = a(e^{iHt} f)$$

For a β-KMS state ω we can compute

$$\omega(a^*(f)\, a(g)) \overset{CAR}{=} \omega(-a(g)\, a^*(f) + \langle g, f \rangle)$$

$$\overset{\text{linear}}{=} -\omega(a(g)\, a^*(f)) + \langle g, f \rangle$$

$$\overset{\text{KMS}}{=} -\omega(\alpha_{-i\beta}(a^*(f))\, a(g)) + \langle g, f \rangle$$

$$= -\omega(a^*(e^{+\beta H} f)\, a(g)) + \langle g, f \rangle$$

By linearity of ω and a^* we thus have

$$\omega\left(a^*\left(\left(1\!\!1 + e^{+\beta H}\right) f\right) a(g)\right) = \langle g, f \rangle$$

As $e^{-\beta H} \geq 0$, $(1\!\!1 + e^{\beta H})$ is invertible and we can set $\xi = (1\!\!1 + e^{+\beta H}) f$, $f = \frac{e^{-\beta H}}{1 + e^{-\beta H}} \xi$

and thus

$$\omega(a^*(\xi)\, a(g)) = \langle g, \frac{e^{-\beta H}}{1 + e^{-\beta H}} \xi \rangle$$

In particular, for the number operator / occupation number in state g

$$N(g) = a^*(g)\, a(g)$$

$$\omega(N(g)) = \langle g, \frac{e^{-\beta H}}{1 + e^{-\beta H}} g \rangle$$

NB: The RHS is computed in the 1-particle HS.

With a similar calculation, one can compute

$$\omega\left(a^*(g_M) \cdots a^*(g_1)\, a(f_1) \cdots a(f_N)\right) = \delta_{MN} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma) \prod_{i=1}^{N} \langle g_i, \frac{e^{-\beta H}}{1 + e^{-\beta H}} f_{\sigma(i)} \rangle$$

This is Wick's theorem.

Obviously, this state is completely determined by the 2-pt function. Such a state (subject to Wick's theorem) is called <u>quasi-free</u>.

$$\omega(\ldots) = \delta_{n,m} \det(\langle f_i, \rho g_j \rangle)$$

for some $0 \leq \rho = \rho^* \leq \mathbb{1}$. (1-particle density op)

Building the GNS-representation on these leads to the Araki-Wyss representation:

$$\mathcal{H}_\rho = \mathcal{F}_-(h) \otimes \mathcal{F}_-(h)$$

$$\Omega_\rho = \Omega_0 \otimes \Omega_0$$

$$a_\rho(f) := \pi_\rho(a(f)) = \underbrace{a_-(\sqrt{1-\rho}\, f)}_{\text{particles}} \otimes 1 + (-1)^N \otimes \underbrace{a_-^*(\sqrt{\rho}\, \bar{f})}_{\text{holes.}}$$

<u>Thm</u> This is quasi-equivalent to Fock iff ρ is trace-class.

non-trivial proof omitted.

Bosons & Bose-Einstein Condensation:

We can try the same calculations for CCR i.e. bosons.

To be able to compare directly with fermions, we will at first assume, we are in a regular representation and have creation and annihilation operators (Weyl operators follow later).

Let us shift the one-particle Hamiltonian by a chemical potential (energy per particle) to $h-\mu$ and define $z := e^{\beta\mu}$ "activity" which we can later adjust to fix the density at a prescribed value ϱ_0.

Let's go

$$\omega(a^*(f)\,a(g)) \overset{\text{KMS}}{=} \omega(a(g)\,a^*(e^{-\beta(h-\mu)}f))$$

$$\overset{\text{CCR}}{=} \omega(a^*(e^{-\beta(h-\mu)}f)\,a(g)) + \langle g, e^{-\beta(h-\mu)}f\rangle$$

$$\overset{\text{iterate } N \text{ times}}{=} \omega\Big(a^*\big(\underbrace{(e^{-\beta(h-\mu)})^N f}_{\displaystyle\downarrow \atop \displaystyle 0 \text{ as long as } \boxed{h-\mu \geq \varepsilon\, \mathrm{id} > 0}}\big)\, a(g)\Big) + \sum_{n=1}^{N} \langle g, (e^{-\beta(h-\mu)})^n f\rangle$$

$$= \Big\langle g, \frac{e^{-\beta(H-\mu)}}{1-e^{-\beta(H-\mu)}} f \Big\rangle$$

& again Wick's theorem.

This is simpler for Weyl operators:

Consider

$$\xi(t) := \omega\big(W(-f)\, W(e^{it(H-\mu)} f)\big)$$

$$= \omega\Big(W\big((-1+e^{it(H-\mu)}) f\big)\Big)\, e^{\frac{i}{2}\operatorname{Im}\langle f, e^{i(H-\mu)t} f\rangle}$$

Define $\eta := (-1+e^{it(H-\mu)}) f$ and obtain (as long as $(-1+e^{it(H-\mu)})$ is invertible)

$$\xi(t) = \omega(W(\eta))\, \exp\Big[-\frac{1}{4}\big\langle \eta, (-1+e^{-i(H-\mu)t})^{-1} \times$$

$$\times \big(e^{i(H-\mu)t} - e^{-i(H-\mu)t}\big) \times$$

$$(-1 + e^{+i(H-\mu)t})\,\eta\rangle$$

Now, analytically continue to $t \to i\beta$ in the expectations

$$-\langle \eta, \cancel{(-1+e^{+\beta(H-\mu)})}\,\cancel{(e^{+\beta(H-\mu)}-1)}(e^{-\beta(H-\mu)}+1)(-1+e^{-\beta(H-\mu)})\eta\rangle$$

i.e.

$$\xi(i\beta) = \omega(W(\eta))\, e^{-\frac{1}{4}\langle \eta, \left(1+2\frac{1}{-1+e^{\beta(H-\mu)}}\right)\eta\rangle}$$

KMS: $\xi(i\beta) = \omega(W(f)\,W(-f)) = 1$

So

$$\omega(W(\eta)) = \tfrac{1}{4}\langle \eta, (1+2\rho)\eta\rangle$$

for

$$\rho = \frac{1}{-1+e^{-\beta(H-\mu)}}$$

Again - we find a quasi-free or Gaussian state

$\log \omega(W(f))$ is quadratic in f, so no truncated correlation functions beyond $n=2$.

But in both CCR calculations, it was crucial that $H-\mu$ was strictly positive.
This is not the case for $H=-\Delta$ on $L^2(\mathbb{R}^n)$.

In that case, there is an additional term projecting on "the 0-mode" "vers".
And for

$$\omega\left(a^*(f)\,a(f)\right) = \cdots + c\,\Big|\underbrace{\int f}_{\langle 1|f\rangle}\Big|^2$$

This is the Bose-Einstein condensate

In this case $\mu<0$ $\quad (z=e^{\beta\mu}<1)$ still saves the day.

In a large but finite volume $|\Lambda|$, the density is given by

$$\varrho(\mu,\beta) = \frac{N}{|\Lambda|} = \frac{\sum_n \omega(a^*(f_n)\, a(f_n))}{|\Lambda|} \quad \text{for some ON basis } f_n$$

$$= \frac{1}{|\Lambda|} \operatorname{tr} \frac{e^{-\beta(H-\mu)}}{1-e^{-\beta(H-\mu)}}$$

Clearly, this goes to ∞ for $\mu \to \inf(\sigma(H))$.

Furthermore, $\frac{\partial \varrho}{\partial \mu} > 0$ and $\lim_{\mu \to -\infty} \varrho = 0$

So we can adjust any density by picking the appropriate $-\infty < \mu < \inf \sigma(H)$.

In infinite volume, we can compute the trace in momentum space:

$$\varrho(\mu,\beta) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \frac{z\, e^{-\beta p^2}}{1-z\, e^{-\beta p^2}}\, d^n p$$

$$\overset{z\leq 1}{\leq} \frac{1}{(2\pi)^n} \int \frac{e^{-\beta p^2}}{1-e^{-\beta p^2}}$$

$$= \frac{1}{(2\pi\sqrt{\beta})^n} \int \frac{e^{-x^2}}{1-e^{-x^2}} \, d^n x$$

goes exponentially to 0 for $|x| \to \infty$.

At $x \approx 0$, $1-e^{-x^2} \approx -x^2$, so this integral is finite for $n>2$!

This suggests a maximum density

$$\rho_c(\beta) = \frac{1}{(2\pi\sqrt{\beta})^n} \int \frac{e^{-x^2}}{1-e^{-x^2}} \, d^n x$$

$$\overset{n=3}{=} \frac{1}{8\pi^{3/2}\sqrt{\beta}} \, \zeta\left(\tfrac{3}{2}\right).$$

How can this be reconciled with the TDL?

It turns out (HW), that for finite $|\Lambda|$, the lowest mode of $-\Delta$ (w/ boundary conditions) and energy γ_1

$$\lim_{\Lambda \to \mathbb{R}^n} \frac{1}{|\Lambda|} \frac{z_\Lambda e^{-\beta\gamma_1}}{1-z_\Lambda e^{-\beta\gamma_1}} = \gamma_0 - \gamma_c.$$

"the remaining density is in the 0-mode".