Easy Vs Hard Problems

Consider the following three distinct class of Hamiltonians written in the first-quantized notation:

(i) $$H = \sum_i \left[\frac{p_i^2}{2m} + V(x_i) \right]$$

(ii) $$H = \sum_{ij} \left[T_{ij} p_i p_j + K_{ij} x_i x_j + V_{ij} (x_i p_j + p_j x_i) \right]$$

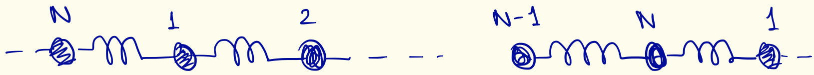
(iii) $$H = \sum_i \left[\frac{p_i^2}{2m} + V(x_i - x_j) \right]$$ where

$V(x_i - x_j)$ is neither linear, nor quadratic in $x_i - x_j$, e.g., $V(x_i - x_j) = (x_i - x_j)^4$

Problems of type (i) are easy because one has to just solve a schrodinger's eqn. for a single particle in potential $V(x)$. They can also be formulated as $H = \sum_\alpha a^\dagger_\alpha a_\alpha \varepsilon_\alpha$ using second quantization. Problems of type (iii) are hard because the interaction term becomes non-quadratic in $a, a^\dagger$. Problems of type (ii) are easy as it is still quadratic in $a, a^\dagger$.

To illustrate type (ii) problems, let us study a simple example:

Consider a system of coupled Harmonic oscillators:



We model it via the following Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} m \omega_0^2 \sum_{i=0}^{N} (\hat{x}_i - \hat{x}_{i+1})^2$$

with $\hat{x}_{N+1} = \hat{x}_1$

The Heisenberg's equations of motion are:

$$\frac{d\hat{p}_i}{dt} = m\omega_0^2 (\hat{x}_{i+1} + \hat{x}_{i-1} - 2\hat{x}_i)$$

$$\Rightarrow m\frac{d^2\hat{x}_i}{dt^2} = m\omega_0^2 (\hat{x}_{i+1} + \hat{x}_{i-1} - 2\hat{x}_i)$$

$\left[k = \frac{2\pi m}{N},\ m = 0 - N-1\right]$

Fourier transforming:

$$\hat{x}_k = \frac{1}{\sqrt{N}} \sum_i \hat{x}_i \, e^{-ik \cdot r_i}$$

(r_i = mean location of $\hat{x}_i$)

$$\Rightarrow \frac{d^2\hat{x}_k}{dt^2} = \omega_0^2 \hat{x}_k (e^{-ik \cdot a} + e^{ika} - 2)$$

$$= -4\omega^2 \sin^2\left(\frac{ka}{2}\right) \hat{x}_k$$

$$\Rightarrow \boxed{\frac{d^2\hat{x}_k}{dt^2} + 4\omega^2 \sin^2\left(\frac{ka}{2}\right) \hat{x}_k = 0}$$

Thus, the system decomposes into N 'normal modes' ($\equiv$ decoupled harmonic oscillators) with frequencies:

$$\omega_k = 2\omega_0 \sin\left(\frac{ka}{2}\right) \qquad k = \frac{2\pi n}{N},$$

$$n = 0, 1, 2, \ldots N-1.$$

Note that $k=0$ mode just corresponds to translating the whole system rigidly (i.e. without any internal motion).

These modes are Goldstone modes! $\equiv$ sound modes / vibrational modes.

At low frequency,

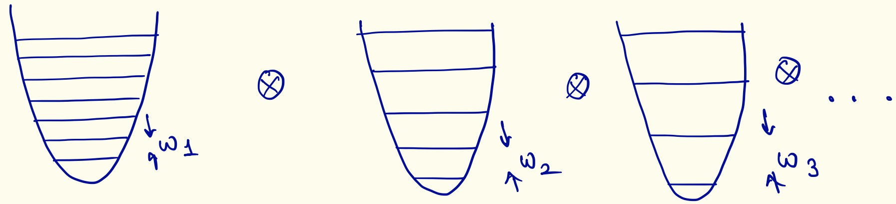
$$\omega_k \sim \omega_0 ka \Rightarrow \omega_k \to 0 \text{ as } k \to 0.$$

Having decomposed the modes into sum of decoupled harmonic oscillators, we can now use our standard technology of a, a^+ operators. Thus,

$$H = \sum_k \omega_k a^+_k a_k$$

where $[a_k, a^+_{k'}] = \delta_{kk'}$.

$H =$



Since each harmonic oscillator mode can have an arbitrary number of excitations, the system is equivalent to a bosonic system with single-particle dispersion:

$$\boxed{\varepsilon_k = \omega_k}$$

You may also show directly that $H = \sum_k \omega_k a^\dagger_k a_k$ by writing x_i, p_i in terms of $a_k, a^\dagger_k$.

$$\hat{x}_i = \frac{1}{\sqrt{N}} \sum_k \hat{x}_k \, e^{ik \cdot r_i}$$

$$= \frac{1}{\sqrt{N}} \sum_k \frac{(a_k + a^\dagger_{-k})}{\sqrt{2 m \omega_k}} \, e^{ik \cdot r_i}$$

$$\hat{p}_i = \frac{1}{\sqrt{N}} \sum_k \hat{p}_k e^{ik \cdot r_i} = \frac{1}{\sqrt{N}} \sum_k \sqrt{\frac{m \omega_k}{2}} \left(a^\dagger_k - a_k \right)$$

Contrast of Physical Properties of Bosons and Fermions.

Two identical fermions can't be in the same state while there is no such restriction for bosons. The truth is even more strikingly different: Bosons prefer to be in the same state while fermions tend to repel each other. Let's see how.

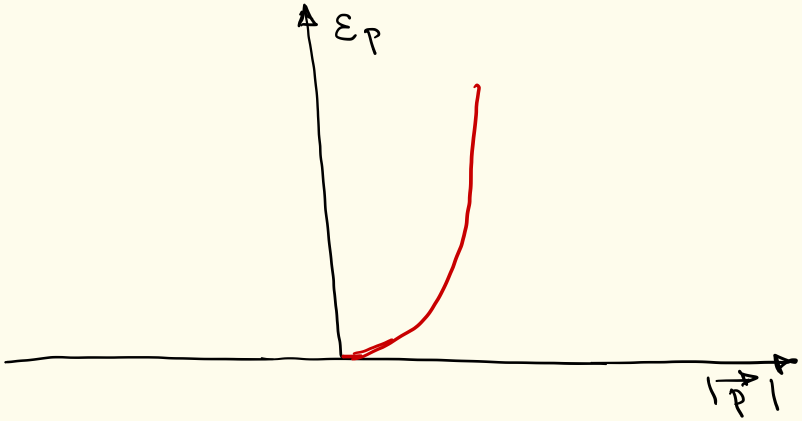
Ground States of Free fermions and Free Bosons:

Free fermions:

Consider the Hamiltonian:

$$H = \sum_p \varepsilon_p a_p^\dagger a_p \quad \text{with}$$

$$\varepsilon_p = \frac{p^2}{2m}.$$



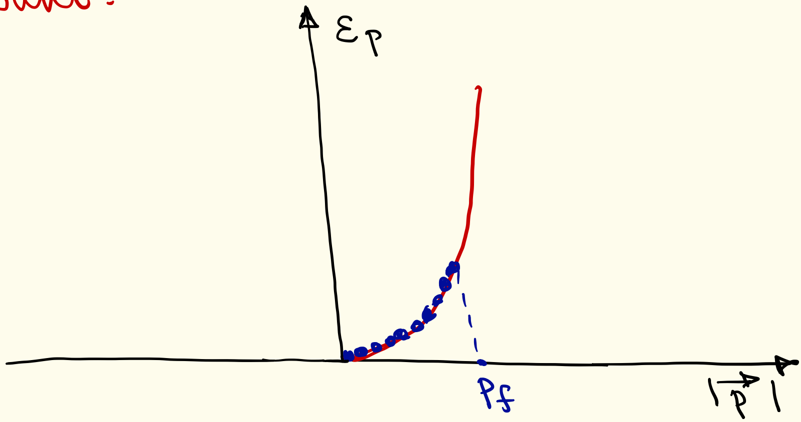
If particles are in a box of dimensions L^d then $\vec{p}$ takes values

$$\hbar\left(\frac{2\pi n_1}{L}, \frac{2\pi n_2}{L}, \ldots \frac{2\pi n_d}{L}\right)$$ in d-dimensions

where n_i are integers in the range 1 to L. As $L \to \infty$, the $\vec{p}$ acts like a continuos variable since Δp = difference between contiguos momenta in energy space $= \frac{2\pi}{L} \to 0$ as $L \to \infty$.

We will then take $\vec{p}$ to be a continuos variable (see pset-2, problem 1 where $\vec{p}$ takes discrete values).

Ground state without taking spin into account:



If there are N fermions (we ignore spin for the moment), they all occupy distinct momenta such that the energy is minimized. Thus, these momenta are contiguous in the energy space.

$$\boxed{\underbrace{|\psi_0\rangle}_{\text{ground state}} = \prod_{|\vec{p}|<p_f} a^{+}(\vec{p}) \underbrace{|0\rangle}_{\substack{\text{No particles} \\ \text{"vacuum"}}}}$$

The crucial thing to note is that p_f is a f^n of particle density and <u>not</u> just particle number. This is obvious on dimension grounds:

$$p_f \sim \frac{\hbar}{\text{inter-particle distance}} \sim \frac{\hbar}{\left[V/N\right]^{1/d}}$$

$$\sim \hbar\, \rho^{1/d}$$

Let's do a more precise calculation:

Number of particles N

$$= \langle \varphi_0 | \hat{N} | \varphi_0 \rangle$$

$$= \langle \varphi_0 | \sum_{\vec{p}} a^+_{\vec{p}}\, a_{\vec{p}} | \varphi_0 \rangle$$

Now $\langle \varphi_0 | a^+_{\vec{p}}\, a_{\vec{p}} | \varphi_0 \rangle = 0$ if $|\vec{p}\,| > |\vec{p}_f|$

$= 1$ if $|\vec{p}\,| \leq |\vec{p}_f|$

$$\Rightarrow \quad N = \sum_{|\vec{p}| < p_f} 1$$

$$= V \int_0^{p_f} \frac{d^d p}{(2\pi)^d}$$

$$= V \frac{p_f^d}{(2\pi)^d} \times \text{Volume of } d\text{-dimensional hypersphere of unit radius.}$$

$$= \frac{V p_f^d}{(2\pi)^d} \frac{\pi^{d/2}}{\Gamma(d/2 + 1)}$$

$$\Rightarrow \quad p_f \propto \left(\frac{N}{V}\right)^{1/d} \quad \text{as expected}$$

When $d = 3$

$$N = \frac{V}{8\pi^3} p_f^3 \frac{4}{3}\pi$$

$$\Rightarrow \quad p_f = \left[6\pi^2 \rho\right]^{1/3}$$

where $\rho = N/V$

With Spin:

Let's study ground state of e^-s which have spin-1/2.

Now, the creation/annihilation operators carry two quantum numbers, $\vec{p}$ and $\sigma = \pm 1/2$ i.e. $a^\dagger(\vec{p}, \sigma)$

For free electrons, the energy eigenvalues are independent of spin:

$$H = \sum_{\vec{p}\,\sigma} \frac{p^2}{2m} a^\dagger(\vec{p}, \sigma)\, a(\vec{p}, \sigma)$$

Thus, the ground state is:

$$\boxed{\underbrace{|\psi_0\rangle}_{\text{ground state}} = \prod_{\substack{|\vec{p}| < p_f \\ \sigma}} a^\dagger(\vec{p}, \sigma) \underbrace{|0\rangle}_{\text{No Particles}}}$$

$$N = \sum_{\vec{p},\sigma} \langle \psi_0 | a^\dagger(\vec{p},\sigma)\, a(\vec{p},\sigma) | \psi_0 \rangle$$

$$= \sum_{\sigma=\pm 1/2} \sum_{\vec{p}} \langle \psi_0 | a^\dagger(\vec{p},\sigma) a(\vec{p},\sigma) | \psi_0 \rangle$$

$$= 2 \times \sum_{|\vec{p}| < p_f} 1$$

$$= \frac{V\, p_f^3}{3\pi^2} \quad \text{in} \quad d = 3.$$

$$\Rightarrow \quad p_f = \left[3\pi^2 \rho \right]^{1/3}$$

Ground State Energy:

$$E_0 = \langle \psi_0 | \hat{H} | \psi_0 \rangle$$

$$= \langle \psi_0 | \sum_{\vec{p}\sigma} a^\dagger(p,\sigma) a(p,\sigma) \frac{p^2}{2m} | \psi_0 \rangle$$

$$= \sum_{\sigma} \sum_{|\vec{p}| < p_f} \frac{p^2}{2m}$$

$$= 2 \frac{V}{(2\pi)^3} \int_0^{p_f} \frac{p^2}{2m} 4\pi p^2 \, dp$$

$$= \left[\frac{p_f^2}{2m} \right] \frac{1}{\pi^2} \frac{p_f^3}{5} V$$

Using $\frac{p_f^3 V}{3\pi^2} = N$ from above, one obtains,

$$\frac{E_0}{N} = \frac{3}{5} \left[\frac{\hbar^2 p_f^2}{2m} \right] = \frac{3}{5} \varepsilon_F \quad \text{where } \varepsilon_F = p_f^2/2m$$

is called "Fermi Energy".

"Fermi- Pressure"

Recall: $dE = T\,dS - P\,dV + \mu\,dN$

$\Rightarrow$ at $T=0$, $P = -\frac{d}{dV} \langle \psi_0 | \hat{H} | \psi_0 \rangle \Big|_N$

$$= -\frac{dE_0}{dV}\Big|_N$$

Using the expression above,

$$E_0 = \frac{3}{5} N \varepsilon_F = \frac{3}{5} N \left[\frac{3\pi^2 N}{V}\right]^{2/3}$$

$$= \frac{3}{5}(3\pi^2)^{2/3} \frac{N^{5/3}}{V^{2/3}}$$

$\Rightarrow$

$$P = \frac{3}{5}(3\pi^2)^{2/3} \frac{N^{5/3}}{2m} \times \frac{2}{3} V^{-5/3}$$

$$= \frac{2}{3}\frac{E}{V}$$

Thus, a fermi gas has a non-zero pressure even at the zero temperature. This is completely different than a classical ideal gas where $P = \rho T = 0$ at $T = 0$.

Correlations in the ground state:

A useful quantity is:

$$G_{\sigma,\sigma'}(r-r') = \langle \psi_0 | a^{+}(\vec{x}, \sigma)\, a(\vec{x}', \sigma') | \psi_0 \rangle$$

i.e. the amplitude for removing a particle from location $\vec{x}'$ with spin σ' returning to location $\vec{x}$ and spin σ.

Since ground state has a definite value of total σ, $G(r-r', \sigma, \sigma')$ is clearly zero when $\sigma \neq \sigma'$. Thus, we don't need two distinct spin indices:

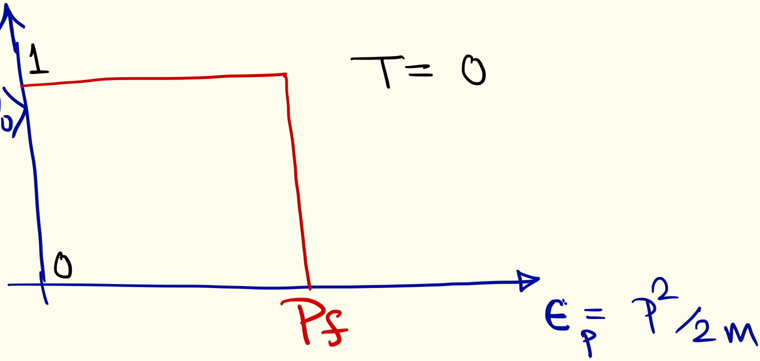
$$G_{\sigma}(r-r') = \langle \psi_0 | a^{+}(\vec{x}, \sigma)\, a(\vec{x}', \sigma) | \psi_0 \rangle$$

$$= \frac{1}{V} \sum_{\vec{p}\vec{p}'} \langle \psi_0 | a^{+}(\vec{p}, \sigma)\, a(\vec{p}', \sigma) | \psi_0 \rangle\, e^{i \vec{p}' \cdot \vec{x}' - i \vec{p} \cdot x}$$

$$= \frac{1}{V} \sum_{\vec{p}} \langle \psi_0 | a^{+}(\vec{p}, \sigma)\, a(\vec{p}, \sigma) | \psi_0 \rangle\, e^{i \vec{p} \cdot (\vec{x}' - \vec{x})}$$

$n_{p\sigma}$

$= \langle \psi_0 | a^\dagger(p,\sigma)\, a(p,\sigma) | \psi_0 \rangle$



$$= \frac{1}{V} \sum_{|\vec{p}|<p_f} e^{i\vec{p}\cdot(\vec{x}'-\vec{x})}$$

$$= \frac{V}{8\pi^3} \frac{1}{V} 2\pi \int_0^{p_f} p^2\, dp \int_0^{\pi} \sin\theta\, d\theta\; e^{ip|\vec{x}'-\vec{x}|\cos\theta}$$

$$= \frac{1}{4\pi^2} \int_0^{p_f} p^2\, dp \int_{-1}^{1} d\mu\; e^{ip|\vec{x}'-\vec{x}|\mu}$$

$$= \frac{1}{4\pi^2} \int_0^{p_f} p^2\, dp \frac{\left(e^{ip|\vec{x}'-x|} - e^{-ip|x'-x|}\right)}{ip|\vec{x}'-\vec{x}|}$$

$$= \frac{1}{4\pi^2} \int_0^{p_f} \frac{2p\, dp\, \sin(pr)}{r}$$

$r = |\vec{x} - \vec{x}'|$

The integral $\int x \sin(\alpha x)\, dx$

$$= -\frac{\cos(\alpha x)\, x}{\alpha} + \int \frac{\cos(\alpha x)}{\alpha}\, dx$$

$$= -\frac{\cos(\alpha x)\, x}{\alpha} + \frac{\sin(\alpha x)}{\alpha^2}$$

$$= \frac{2}{4\pi^2 r}\left[-\frac{\cos(pr)\, p}{r} + \frac{\sin(pr)}{r^2}\right]\Bigg|_0^{p_f}$$

$$= \frac{2}{4\pi^2}\left[-\frac{\cos(p_f r)\, p_f}{r^2} + \frac{\sin(p_f r)}{r^3}\right]$$

define $p_f r = y$

$$= \frac{2 p_f^3}{4\pi^2}\left[\frac{-\cos(y)\, y + \sin(y)}{y^3}\right]$$

Now recall $p_f^3 = 3\pi^2 \rho$

$$\Rightarrow G_r(\vec{r}-\vec{r}\,') = \frac{3}{2}\rho\left[\frac{\sin(y) - y\cos(y)}{y^3}\right]$$

Thus G shows oscillations at scale p_f^{-1} and decays in a <u>power-law</u> fashion.

The power-law originates from the fact that $\langle n_{p\sigma} \rangle$ is singular in the ground state. The Fourier transform of $G(r-r')$ is also singular at

$$G(\vec{q}) = \frac{1}{\sqrt{V}} \int_{\vec{r}} G(\vec{r})\, e^{+i\vec{q}\cdot\vec{r}}\, d^3r$$

$$\sim \frac{\int d^3r}{\sqrt{V}} \int_{|p|<p_f} d^3p\; e^{-i\vec{p}\cdot\vec{r} + i\vec{q}\cdot\vec{r}}$$

$$\sim \int_{|p|<p_f} \delta(\vec{p}-\vec{q})\, d^3p$$

$$= \begin{cases} 0 & \text{if } |\vec{q}| > p_f \\ 1 & \text{if } |\vec{q}| < p_f \end{cases}$$