Free Fermi gas

N noninteracting electrons at $T=0$

$$\hat{H} = \sum_{\bar{k}\sigma} \frac{\hbar^2 \bar{k}^2}{2m} a^+_{\bar{k}\sigma} a_{\bar{k}\sigma} = \sum_{\bar{k}\sigma} \epsilon_{\bar{k}} \hat{n}_{\bar{k}\sigma}$$

BASIS STATES $\{|\bar{k},\sigma\rangle\}$ $\left(\langle \bar{r}\sigma' | \bar{k}\sigma\rangle = \delta_{\sigma\sigma'} \frac{1}{\sqrt{V}} e^{i\bar{k}\bar{r}}\right)$

(PERIODIC B.C.) $V = L^3$

$$\vec{k} = \frac{2\pi}{L}\vec{n}, \quad \bar{n} = (n_x, n_y, n_z) \quad n_i \in \mathbb{Z}$$

STATES ARE ORDERED AS FOLLOWS:

$|\bar{k}_1,\uparrow\rangle, |\bar{k}_1,\downarrow\rangle, |\bar{k}_2,\uparrow\rangle, |k_2,\downarrow\rangle, \dots$

SUCH THAT $\epsilon_{\bar{k}_1} \le \epsilon_{\bar{k}_2} \le \epsilon_{\bar{k}_3} \le \dots$

Ground state:

$$|FS\rangle = a^+_{\bar{k}_1\uparrow} a^+_{\bar{k}_1\downarrow} a^+_{2\bar{k}\uparrow} a^+_{2\bar{k}\downarrow} \dots a^+_{\bar{k}_{\frac{N}{2}}\uparrow} a^+_{\bar{k}_{\frac{N}{2}}\downarrow} |0\rangle$$

(FERMI sea)

The highest energy of an occupied 1-body state $\to$ Fermi energy (ϵ_F)

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

$$k_F = \frac{1}{\hbar}\sqrt{2m\epsilon_F} \quad \to \text{Fermi wavevector}$$

$$v_F = \frac{\hbar k_F}{m} \quad \to \text{Fermi velocity}$$

$$T_F = \frac{\epsilon_F}{k_B} \quad \to \text{Fermi temperature}$$

We are interested in the thermodynamic limit $N\to\infty$, $L\to\infty$, $n = \frac{N}{L^3} = \text{const}$.

$$\hat{n}_{\bar{k}\sigma}|FS\rangle = \Theta(k_F - |\bar{k}|)|FS\rangle$$

$$\frac{1}{V}N = \frac{1}{V}\langle FS|\sum_{\bar{k}\sigma}\hat{n}_{\bar{k}\sigma}|FS\rangle \xrightarrow[\substack{N\to\infty \\ n=\text{const}}]{V\to\infty} \frac{1}{V}\frac{V}{(2\pi)^3}\sum_\sigma\int d^3k\, \Theta(k_F - |\bar{k}|)\langle FS|FS\rangle$$

$$n = \frac{2}{(2\pi)^3}\int_0^{k_F} 4\pi\, dk\, k^2 = \frac{2}{(2\pi)^3}\frac{4}{3}\pi k_F^3 = \frac{1}{3\pi^2}k_F^3$$

$$k_F = (3\pi^2 n)^{\frac{1}{3}}$$

E.G. Copper $n \simeq 8.5\cdot 10^{28}\, m^{-3}$

$\hookrightarrow k_F \approx 14\cdot 10^9\, m^{-1}$

$\epsilon_F \simeq 10^{-18}\, J \simeq 7\, eV$

$T_F \approx 10^5\, K$!!!

$v_F \simeq 10^6\, \frac{m}{s} \ll c \Rightarrow$ (nonrelativistic system)

Internal energy (at $T=0$)

$$E^{(0)} = \langle FS|\hat{H}|FS\rangle = \sum_{\vec{k}\sigma} \frac{\hbar^2 k^2}{2m} \langle FS|\hat{n}_{\vec{k}\sigma}|FS\rangle =$$

$$= 2\frac{V}{(2\pi)^3}\frac{\hbar^2}{2m}\int d^3k\, k^2\, \Theta(k_F-k) = 2\frac{V}{(2\pi)^3}\frac{\hbar^2}{2m}4\pi\int_0^{k_F} dk\, k^4 =$$

$$= \frac{V}{5\pi^2}\frac{\hbar^2}{2m}k_F^3 = \frac{V}{5\pi^2}\epsilon_F k_F^3 = \frac{3}{5}N\epsilon_F \Rightarrow \frac{E^{(0)}}{N} = \frac{3}{5}\epsilon_F = \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2)^{\frac{2}{3}}n^{\frac{2}{3}}$$

$$E^{(0)} = \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2)^{\frac{2}{3}}N^{5/3}V^{-\frac{2}{3}}$$

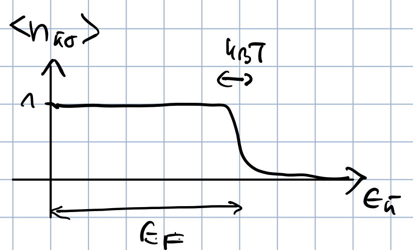
Pressure: $p = -\left(\frac{\partial E^{(0)}}{\partial V}\right)_N = \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2)^{\frac{2}{3}}\frac{2}{3}n^{5/3} \simeq 10^6\,\text{atm}$!!!

Perfect gas (classical) $p = nRT \overset{T=0}{=} 0$

Finite temperature: Fermi-Dirac distribution

$$\langle n_{\vec{k}\sigma}\rangle = \frac{1}{e^{\beta(\epsilon_{\vec{k}}-\mu)}+1} \xrightarrow{T\to 0} \Theta(\epsilon_F-\epsilon_{\vec{k}})$$

$$(\beta^{-1} = k_B T) \qquad \epsilon_F = \mu(T=0)$$



Time evolution of quantum systems

Schrödinger picture

state vectors do depend on time $|\psi(t)\rangle$

$$i\hbar\partial_t|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

If $\hat{H}$ does not depend on time, we obtain

$$|\psi(t)\rangle = e^{-i\frac{\hat{H}}{\hbar}t}\underbrace{|\psi(t=0)\rangle}_{|\psi_0\rangle}$$

recall: $$f(\hat{A}) = \sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}\hat{A}^n$$

Heisenberg picture

$$\langle \psi'(t) | A | \psi(t) \rangle = \langle \psi_0' | \overbrace{e^{\frac{i\hat{H}t}{\hbar}} A e^{-i\frac{\hat{H}t}{\hbar}}}^{:= A(t)} | \psi_0 \rangle$$

Assume $\hat{H}$ does not depend on t

$$A(t) := e^{\frac{iHt}{\hbar}} A e^{-\frac{iHt}{\hbar}}$$

$$|\psi_0\rangle = e^{\frac{iHt}{\hbar}} |\psi(t)\rangle$$

States do not depend on t in Heisenberg picture.

Time evolution of $A(t)$

$$\frac{dA(t)}{dt} = \dot{A}(t) = e^{i\frac{Ht}{\hbar}} \left(\frac{iH}{\hbar} A + \frac{\partial A}{\partial t} - \frac{i}{\hbar} AH \right) e^{-i\frac{Ht}{\hbar}}$$

$$\dot{A}(t) = \frac{i}{\hbar} [H, A(t)] + (\partial_t A)(t)$$

$$X(t) \to e^{\frac{iHt}{\hbar}} X e^{-\frac{iHt}{\hbar}}$$

Interaction picture

$$H = H_0 + V$$

$\hookrightarrow$ time-independent, known eigenstates and eigenvalues

$$\hat{A}(t) = e^{i\frac{H_0}{\hbar}t} A e^{-i\frac{H_0}{\hbar}t}$$

$$|\hat{\psi}(t)\rangle = e^{i\frac{H_0 t}{\hbar}} |\psi(t)\rangle$$

For $V = 0$ Heisenberg and interaction pictures are equivalent.

Evolution of $|\hat{\psi}(t)\rangle$:

$$i\partial_t |\hat{\psi}(t)\rangle = i\partial_t \left(e^{i\frac{H_0 t}{\hbar}}\right) |\psi(t)\rangle + e^{i\frac{H_0 t}{\hbar}} i\partial_t |\psi(t)\rangle =$$

$$= e^{i\frac{H_0 t}{\hbar}}\left(-\frac{H_0}{\hbar}\right)|\psi(t)\rangle + e^{i\frac{H_0 t}{\hbar}}\frac{H}{\hbar}|\psi(t)\rangle =$$

$$= e^{i\frac{H_0 t}{\hbar}}\underbrace{\left(-\frac{H_0}{\hbar}+\frac{H}{\hbar}\right)}_{=\frac{V}{\hbar}}|\psi(t)\rangle = \underbrace{e^{i\frac{H_0 t}{\hbar}}\frac{1}{\hbar}V e^{-i\frac{H_0 t}{\hbar}}}_{\frac{1}{\hbar}\hat{V}(t)}|\hat{\psi}(t)\rangle$$

$$i\hbar\,\partial_t|\hat{\psi}(t)\rangle = \hat{V}(t)\,|\hat{\psi}(t)\rangle \quad (*)$$

Time evolution (in interaction representation) should be given by a unitary operator depending (only) on $\hat{V}(t)$. Can we find it?

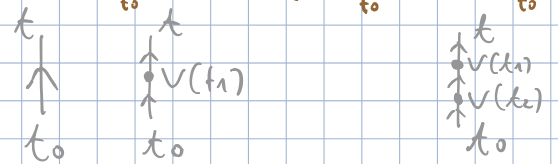
$$|\hat{\psi}(t)\rangle = \underbrace{\hat{U}(t,t_0)}_{=\,?}|\hat{\psi}(t_0)\rangle \qquad U(t_0,t_0) = 1$$

$$i\partial_t|\hat{\psi}(t)\rangle = i\partial_t\left(\hat{U}(t,t_0)|\hat{\psi}(t_0)\rangle\right) \overset{(*)}{=} \frac{1}{\hbar}\hat{V}(t)\,\hat{U}(t,t_0)|\hat{\psi}(t_0)\rangle$$

$$\Rightarrow\ i\partial_t\hat{U}(t,t_0) = \frac{1}{\hbar}\hat{V}(t)\,\hat{U}(t,t_0) \qquad \left(\text{and } \hat{U}(t_0,t_0) = \mathbb{1}\right)$$

Integrating: $\hat{U}(t,t_0) = \frac{1}{i\hbar}\int_{t_0}^{t} dt'\,\hat{V}(t')\,\hat{U}(t',t_0) + 1$ (integral eq. for $\hat{U}(t,t_0)$) Iterate...

$$\hat{U}(t,t_0) = 1 + \frac{1}{i\hbar}\int_{t_0}^{t} dt_1\,\hat{V}(t_1) + \frac{1}{(i\hbar)^2}\int_{t_0}^{t} dt_1\,\hat{V}(t_1)\int_{t_0}^{t_1} dt_2\,\hat{V}(t_2) + \dots$$



 represents evolution given by H_0 (no V)

- look at the 2nd term in our expansion: $\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\,\hat{V}(t_1)\hat{V}(t_2) =$

$$= \frac{1}{2}\left[\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\,\hat{V}(t_1)\hat{V}(t_2) + \int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1\,\hat{V}(t_2)\hat{V}(t_1)\right] =$$

$$= \frac{1}{2}\left[\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2\,\hat{V}(t_1)\hat{V}(t_2)\,\Theta(t_1-t_2) + \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2\,\hat{V}(t_2)\hat{V}(t_1)\,\Theta(t_2-t_1)\right] =$$

$$= \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2\; T\left[\hat{V}(t_1)\hat{V}(t_2)\right]$$

$$T\left[\hat{V}(t_1)\hat{V}(t_2)\right] := \hat{V}(t_1)\hat{V}(t_2)\,\Theta(t_1-t_2) + \hat{V}(t_2)\hat{V}(t_1)\,\Theta(t_2-t_1)$$

$\longrightarrow$ time-ordering operator

- look at the 3rd term in our expansion:

$$\int_{t_0}^{t} dt_1\,\hat{V}(t_1)\int_{t_0}^{t_1} dt_2\,\hat{V}(t_2)\int_{t_0}^{t_2} dt_3\,\hat{V}(t_3) = \frac{1}{3!}\left[\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3\,\hat{V}(t_1)\hat{V}(t_2)\hat{V}(t_3) + \left\{\begin{array}{l}\text{5 analogous terms}\\ \text{with the dummy}\\ \text{variables } \{t_1,t_2,t_3\}\\ \text{permuted}\end{array}\right\}\right] =$$

$$= \frac{1}{3!}\left[\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_3\,\Theta(t_1-t_2)\,\Theta(t_2-t_3)\,\hat{V}(t_1)\hat{V}(t_2)\hat{V}(t_3) + \{\text{5 terms}\dots\}\right] =$$

$$= \frac{1}{3!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \int_{t_0}^{t} dt_3\; T\left[\hat{V}(t_1)\hat{V}(t_2)\hat{V}(t_3)\right]$$

• the n-th term of this expansion:

$$\int_{t_0}^{t} dt_1 \hat{V}(t_1) \int_{t_0}^{t_1} dt_2 \hat{V}(t_2) \dots \int_{t_0}^{t_{n-1}} dt_n \hat{V}(t_n) = \frac{1}{n!} \sum_{P} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \dots \int_{t_0}^{t} dt_n \hat{V}(t_{P_1}) \hat{V}(t_{P_2}) \dots \hat{V}(t_{P_n}) \theta(t_{P_1} - t_{P_2}) \dots \theta(t_{P_{n-1}} - t_{P_n})$$

$$= \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \dots \int_{t_0}^{t} dt_n \, T\left[\hat{V}(t_1) \hat{V}(t_2) \dots \hat{V}(t_n)\right]$$

$$T\left[\hat{V}(t_1) \hat{V}(t_2) \dots \hat{V}(t_n)\right] := \sum_{P} \hat{V}(t_{P_1}) \hat{V}(t_{P_2}) \dots \hat{V}(t_{P_n}) \, \theta(t_{P_1} - t_{P_2}) \theta(t_{P_2} - t_{P_3}) \dots \theta(t_{P(n-1)} - t_{P_n})$$

→ time ordering (chronological) operator

We obtain: $\underline{\mathcal{U}(t, t_0) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} dt_1 \dots \int_{t_0}^{t} dt_n \, T\left[\hat{V}(t_1) \dots \hat{V}(t_n)\right] = \mathcal{T} e^{-\frac{i}{\hbar} \int_{t_0}^{t} dt' \hat{V}(t')}}$

For $\hat{V}(t)$ "sufficiently small": $\hat{\mathcal{U}}(t, t_0) \simeq 1 + \frac{1}{i\hbar} \int_{t_0}^{t} dt' \hat{V}(t')$