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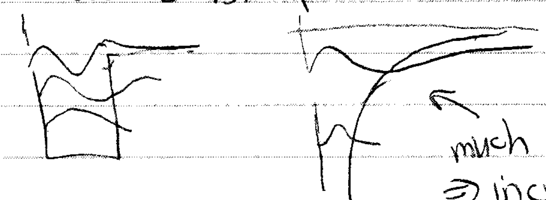
Monday 880.05 Class

Comments on PS#2

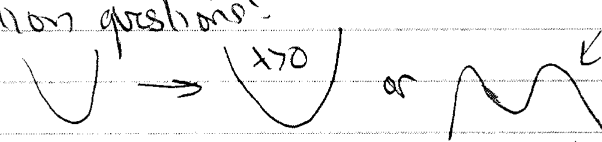
1. MATLAB sandbox
   - norm(E+F−E,1) > 0 ? If adding F doesn't change E, then beyond machine precision ($1+\epsilon=1$ for mch. prec. ϵ)
   - If you use randn to check terms, then about 54. If you shift to [0,1], then ~121, like uniform!

2. SVM
   - Coulomb vs. square well w/ excited states



   - optimize lowest first, then next, etc. Why not this not screw up the first state?

3. Acceptance rate roughly 50% (compromise).
   - Thermalization questions?
   - Physics



   integration over all x will find eventually. Metastable?

4. $U = e^{-i\frac{2\pi q k}{N_T}}$ ⇒ [q,k] = meshgrid(1:Nt,1:Nt) e.g. Nt=10

   U = exp(-i*2*pi/Nt*q.*k)

$N_t=3$ $q=\begin{pmatrix}1&2&3\\1&2&3\\1&2&3\end{pmatrix}$ $k=\begin{pmatrix}1&1&1\\2&2&2\\3&3&3\end{pmatrix}$ $q.*k=\begin{pmatrix}1&2&3\\2&4&6\\3&6&9\end{pmatrix}$

translational invariance $\frac{1}{N_T}\sum_{k,j} e^{i\frac{2\pi}{N_T}qk} B_{kj} e^{-i\frac{2\pi}{N_T}jq'}$

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4. (cont) Now think that translational invariance is about k, j, or $j-k$.

$$\Rightarrow j=(j-k)+k \Rightarrow \frac{1}{N_\tau}\sum_k e^{i\frac{2\pi}{N_\tau}(q-q')k} \sum_j e^{-i\frac{2\pi}{N_\tau}(j-k)} \underbrace{A(j-k)}_{\text{independent of } k\text{. Why?}}$$

$\leftarrow \delta_{qq'}$

<u>Problem</u>! An eigenvalue of A is zero with eigenvector $\begin{pmatrix}1\\1\\1\end{pmatrix}$

$$\begin{pmatrix} +2 & -1 & 0 & -1 \\ -1 & 2 & 0 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{pmatrix}\begin{pmatrix}1\\1\\1\\1\end{pmatrix} = 0\begin{pmatrix}1\\1\\1\\1\end{pmatrix}$$

A "zero mode" is common $\Rightarrow \det(A)=0$ and A^{-1} doesn't exist!

How to fix? Here, add $+a$ to diagonal $(+ax^2)$

5. Revisit G^0 from last week and look at properties.
 · see me about FT issues!

$$Z=\int \mathcal{D}(\psi^\dagger\psi)e^{-S_E}$$

On left board: $S_E = \int d\tau \int d^3x \left[\psi^\dagger_\alpha(x)\left(\frac{\partial}{\partial\tau}-\frac{\nabla^2}{2m}-\mu\right)\psi_\alpha(x) - \frac{\lambda}{2}\psi^\dagger_\alpha(x)\psi^\dagger_\beta(x)\psi_\beta(x)\psi_\alpha(x)\right]$

$$G^{0-1}G^0=1 \Rightarrow \delta_{\alpha\beta}\left(\frac{\partial}{\partial\tau}-\frac{\nabla^2}{2m}-\mu\right)G^0_{\beta\gamma}(\vec{x}\tau;\vec{x}'\tau') = \delta_{\alpha\gamma}\,\delta^3(\vec{x}-\vec{x}')\,\delta(\tau-\tau')$$

with

$$G^0_{\alpha\beta}(\vec{x}0;\vec{x}'\tau') = -G^0_{\alpha\beta}(\vec{x}\beta;\vec{x}'\tau')$$

Claim:

$$G^0_{\beta\gamma}(\vec{x}\tau;\vec{x}'\tau') = \delta_{\beta\gamma}\int\frac{d^3k}{(2\pi)^3}e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}e^{-(\epsilon^0_k-\mu)(\tau-\tau')}\left[\theta(\tau-\tau'-\eta)(1-n^0_k) - \theta(\tau'-\tau+\eta)n^0_k\right]$$

$\leftarrow$ or $\left(\frac{1}{V}\sum_k\right)$

in case $\tau=\tau'$, we know which one to pick.

where $n^0_k = \dfrac{1}{e^{\beta(\epsilon^0_k-\mu)}+1}$ and $\epsilon^0_k \equiv \dfrac{\hbar^2 |k|^2}{2m}$ (fermions)

$$\frac{Z}{Z_0} = \left.\frac{Z[\eta_\alpha,\eta^\dagger_\alpha]}{Z_0}\right|_{\eta=\eta^\dagger=0} = \left. e^{\int_0^\beta d\tau\int d^3x\,\frac{\lambda}{2}\left(\frac{\delta}{\delta\eta_\alpha(x)}\frac{\delta}{\delta\eta_\beta(x)}\frac{-\delta}{\delta\eta^\dagger_\beta(x)}\frac{-\delta}{\delta\eta^\dagger_\alpha(x)}\right)} e^{\int \eta^\dagger_\gamma G^0_{\gamma\delta}\eta_\delta}\right|_{\eta=\eta^\dagger=0}$$

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- Let's evaluate the trace defining Z_0 using the occupation number basis. In general, these are not eigenstates of $\hat{H}$, but let's start with

$$\boxed{\hat{H} \to \hat{H}_0 = \sum_i \epsilon_i a_i^\dagger a_i \qquad \hat{N} = \sum_i a_i^\dagger a_i}$$

where i runs over the single-particle quantum numbers (e.g. $\vec{k}, \alpha$ for fermions in a box).

- We'll see that the trace is easy to evaluate in this case. This, in turn, will lead to a strategy for evaluating the more general case.

- In the occupation number basis, we don't sum over E_{jN} and N, but over $n_1, n_2, \ldots$ for "modes" (single-particle states) $1, 2, 3, \ldots$

$$\boxed{\begin{aligned} Z_0 = \operatorname{Tr} e^{-\beta(\hat{H}_0 - \mu\hat{N})} &= \sum_{n_1 \cdots n_\infty} \langle n_1 \cdots n_\infty | e^{\beta(\mu\hat{N} - \hat{H}_0)} | n_1 \cdots n_\infty \rangle \\ &= e^{-\beta\Omega_0(T,V,\mu)} \end{aligned}}$$

- Recall that $|n_1 \cdots n_\infty\rangle = |n_1\rangle|n_2\rangle \cdots$
- For bosons, each $n_i = 0, 1, 2, \ldots \infty$ ("i" labels the mode) for fermions, each $n_i = 0$ or 1

$$\Rightarrow \boxed{\hat{H}_0 |n_1 \cdots n_\infty\rangle = \sum_i \epsilon_i a_i^\dagger a_i |n_1 \cdots n_\infty\rangle = \sum_i n_i \epsilon_i |n_1 \cdots n_\infty\rangle}$$

$$\boxed{\hat{N} |n_1 \cdots n_\infty\rangle = \sum_i n_i |n_1 \cdots n_\infty\rangle}$$

- Note that $[\hat{n}_i, \hat{n}_j] = 0$ for all i, j, which means we can exponentiate these results.

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Plugging in;

$$Z_0 = \sum_{n_1 \cdots n_\infty} e^{-\beta \sum_i (\epsilon_i - \mu) n_i} = \left(\sum_{n_1=0}^{\infty \text{ or } 1} e^{-\beta(\epsilon_1-\mu)n_1} \right) \left(\sum_{n_2=0}^{\infty \text{ or } 1} e^{-\beta(\epsilon_2-\mu)n_2} \right) \cdots \left(\cdots \right)$$

boson or fermion; only 1 μ!

bosons: $n_i = 0, 1, 2, \ldots$

$$\boxed{\sum_{n_i=0}^{\infty} e^{-\beta(\epsilon_i-\mu)n_i} = 1 + e^{-\beta(\epsilon_i-\mu)} + e^{-2\beta(\epsilon_i-\mu)} + \ldots \quad \text{(bosons)} = \frac{1}{1-e^{-\beta(\epsilon_i-\mu)}} \quad \text{geometric series!}}$$

fermions: $n_i = 0, 1$

$$\boxed{\sum_{n_i=0}^{1} e^{-\beta(\epsilon_i-\mu)n_i} = 1 + e^{-\beta(\epsilon_i-\mu)} \quad \text{(fermions)}}$$

$$\boxed{\Rightarrow \Omega_0(T,V,\mu) = -\frac{1}{\beta}\ln Z_0 = \begin{cases} +\dfrac{1}{\beta}\displaystyle\sum_{i=1}^{\infty} \ln\left(1-e^{-\beta(\epsilon_i-\mu)}\right) & \text{bosons} \\ -\dfrac{1}{\beta}\displaystyle\sum_{i=1}^{\infty} \ln\left(1+e^{-\beta(\epsilon_i-\mu)}\right) & \text{fermions} \end{cases}}$$

$\Rightarrow$ just two little sign differences!

bosons:

$$\boxed{\langle N \rangle = -\frac{\partial}{\partial\mu}\Omega_0 = -\frac{1}{\beta}\sum_{i=1}^{\infty} \frac{1}{1-e^{-\beta(\epsilon_i-\mu)}}\left(-e^{-\beta(\epsilon_i-\mu)}\right)(+\beta) = \sum_{i=1}^{\infty}\frac{1}{e^{\beta(\epsilon_i-\mu)}-1} \equiv \sum_{i=1}^{\infty} n_i^0 \quad \text{(bosons)}}$$

where n_i^0 is the mean occupation number in the i^{th} state.

Can μ take on any value?

fermions:

$$\boxed{\langle N \rangle = -\frac{\partial}{\partial\mu}\Omega_0 = -\left(-\frac{1}{\beta}\sum_{i=1}^{\infty}\frac{1}{1+e^{-\beta(\epsilon_i-\mu)}} e^{-\beta(\epsilon_i-\mu)}\beta\right) = +\sum_{i=1}^{\infty}\frac{1}{e^{\beta(\epsilon_i-\mu)}+1} \equiv \sum_{i=1}^{\infty} n_i^0 \quad \text{(fermions)}}$$

$\Rightarrow n_i^0 = \left(e^{\beta(\epsilon_i-\mu)}+1\right)^{-1}$ for fermions.

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Example: non-interacting Fermi gas with degeneracy ν in a large box of volume V

$$\Rightarrow \boxed{\epsilon_i \to \epsilon_p = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}}$$

and $$\boxed{\sum_i \xrightarrow[\substack{V\to\infty \\ N\to\infty}]{} \nu V \int \frac{d^3k}{(2\pi)^3}}$$

So $$\boxed{\begin{aligned}\Omega_0(V,T,\mu) &= -\frac{1}{\beta}\sum_i \ln\left(1+e^{-\beta(\epsilon_i-\mu)}\right) \\ &= -\frac{\nu}{\beta}\frac{V}{(2\pi)^3}\int d^3k \ln\left(1+e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}\right)\end{aligned}}$$

- note that the integrand is well-defined and bounded at both small and large k:

$k\to 0$, $k^2\ln\left(1+e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}\right) \to k^2\ln\left(1+e^{\beta\mu}\right) \to 0$

$k\to\infty$, $k^2\ln\left(1+e^{-\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}\right) \to k^2\ln\left(1+e^{-\beta\frac{\hbar^2k^2}{2m}}\right) \to k^2 e^{-\beta\frac{\hbar^2k^2}{2m}} \to 0$

- It's easier to evaluate the integral with $\epsilon = \frac{\hbar^2k^2}{2m}$ as the integration variable:

$$\Rightarrow d\epsilon = \frac{\hbar^2}{m}k\,dk \quad \text{and} \quad k^2dk = \left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{2m}{\hbar^2}\frac{1}{2}\epsilon^{1/2}d\epsilon$$

$$\Rightarrow \boxed{\Omega_0 = -\frac{\nu}{\beta}\frac{V}{8\pi^3}\underbrace{4\pi}_{\text{angular integration}}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{1}{2}\int_0^\infty d\epsilon\, \epsilon^{1/2}\ln\left(1+e^{\beta(\mu-\epsilon)}\right)}$$

It is useful to write this in another form by integrating by parts [$v=\ln(1+e^{\beta(\mu-\epsilon)}) \to dv=(1+e^{\beta(\mu-\epsilon)})^{-1}e^{\beta(\mu-\epsilon)}(-\beta)\,d\epsilon$ and $du=\epsilon^{1/2}d\epsilon \to u=\frac{2}{3}\epsilon^{3/2}$ and the surface term vanishes at $\epsilon=0$ and $\epsilon=\infty$]

$$\Rightarrow \boxed{\Omega_0 = PV = \frac{\nu V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{2}{3}\int_0^\infty d\epsilon\,\frac{\epsilon^{3/2}}{e^{\beta(\epsilon-\mu)}+1}}$$

which gives us the pressure directly.

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· We can find N directly from

$$\boxed{N = \sum_i n_i^0 = \sum_i \frac{1}{e^{\beta(\epsilon_i-\mu)}+1} \longrightarrow + \frac{\nu V}{(2\pi)^3}\int d^3k \, \frac{1}{e^{\beta(\epsilon_k-\mu)}+1} = \frac{\nu V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty d\epsilon \, \frac{\epsilon^{1/2}}{e^{\beta(\epsilon-\mu)}+1}}$$

or from $N = -\frac{\partial \Omega_0}{\partial \mu}$ (use the first version with the ln)

· To find the energy, we can find S from $S = -\left(\frac{\partial \Omega}{\partial T}\right)_{V\mu}$ (recalling $\beta = 1/k_BT$) and then using $E = TS - PV + \mu N$.
Or we can find it directly (in this case) as we did with N:

$$\boxed{E = \sum_i n_i^0 \epsilon_i \longrightarrow \frac{\nu V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)\int_0^\infty d\epsilon \, \frac{\epsilon^{3/2}}{e^{\beta(\epsilon-\mu)}+1}}$$

Comparing the E and Ω_0 equations, we find the "equation of state"

$$\boxed{PV = \frac{2}{3}E}$$

· See Fetter + Walecka exerpts for details of fermions at low temperature and for bosons.

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Aside: consider the fermion occupation number further

$$\boxed{n_i^\circ = \frac{1}{e^{\beta(\epsilon_i-\mu)}+1}}$$

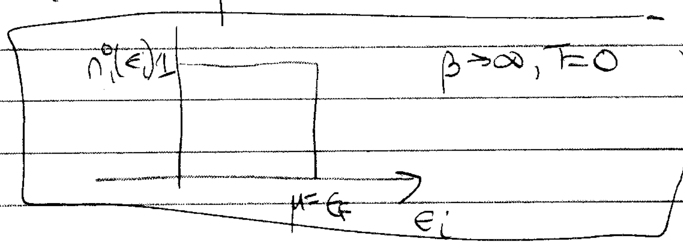
- Since $e^x \geq 0$, $n_i^\circ \leq 1$ (which is good, since we're averaging 0's and 1's, but it means that any μ is possible, unlike the boson case).

- Consider the high temperature ($\beta \to 0$) and low temperature ($\beta \to \infty$) limits of n_i°.

$\beta \to \infty$: if $\epsilon_i - \mu > 0 \Rightarrow e^{\beta(\epsilon_i-\mu)} \to \infty \Rightarrow n_i^\circ \to 0$

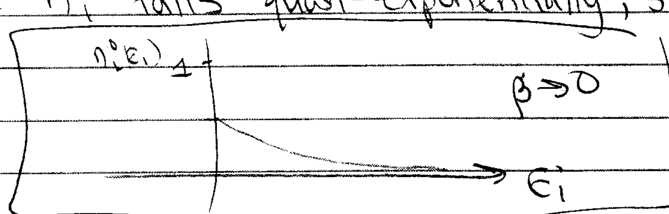
if $\epsilon_i - \mu < 0 \Rightarrow e^{\beta(\epsilon_i-\mu)} \to 0 \Rightarrow n_i^\circ \to 1$

so $n_i^\circ(\epsilon_i) \xrightarrow{\beta\to\infty} \theta(\mu - \epsilon_i)$ and we fill levels up to $\mu = \epsilon_F$



Note that this limit applied to N and E reproduces our previous non-interacting ground state results.

$\beta \to 0$ if $\beta\mu \ll 1$, then μ does not have much of an effect, and $n_i^\circ(\epsilon_i)$ is significant until $\beta\epsilon_i \gg 1$. That means that n_i° falls quasi-exponentially, starting at $n_i^\circ = .5$:



In between, the behavior interpolates between these extremes