November, 2012

Question: for T=0 ground state of a general interacting many electron system connected to an electron reservoir, what is energy versus electron number where electron number can be non-integer. What does it mean and how to do it?

We use density matrix in grand canonical formulation

$$\hat{T} = \exp\left(-\beta(\hat{\mathcal{H}} - \mu\hat{N})\right)/Z \qquad \text{Let } Z = e^{-\beta\alpha}$$

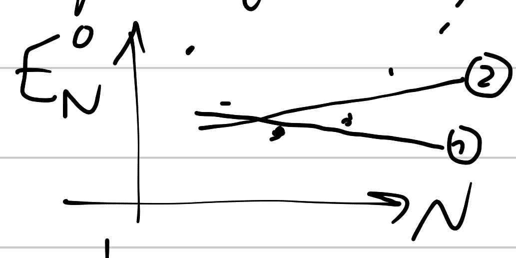
$$= \exp\left(-\beta(\hat{\mathcal{H}} - \mu\hat{N} - \alpha)\right) \qquad \langle\hat{\theta}\rangle \equiv \mathrm{tr}(\hat{T}\hat{\theta})$$

$$= \sum_N \sum_s |Ns\rangle\langle Ns| \exp\left(-\beta(E_N^s - \mu N - \alpha)\right)$$

As $\beta \to \infty$, for fixed N only ground state $s=0$ survives

$$\hat{T} \to \sum_N |N0\rangle\langle N0| \exp\left(-\beta(E_N^0 - \mu N - \alpha)\right)$$

Now consider $d_N = E_N^0 - \mu N - \alpha$. As a function of N, d_N must have a minimum value otherwise the sum won't converge. This means E_N^0 must be concave-up as a function of N (since μ & α can take on various values).



Case 1: single minimum of d_N for $N = \bar{N}$.

Then $\lim_{\beta\to\infty} \begin{cases} Z = e^{-\beta d_{\bar{N}}} \\ \hat{T} = |\bar{N}0\rangle\langle\bar{N}0| \end{cases}$

so $\langle\hat{N}\rangle = \bar{N} = \text{integer}$

$\langle\hat{\mathcal{H}}\rangle = E_{\bar{N}}^0$

Graphical construction is to draw line $\mu N + \alpha$ & d_N is how far E_N^0 is above line.

Case 2: two equal & consecutive minima for $\bar{N}$ & $\bar{N}+1$.

$\langle\hat{\mathcal{H}}\rangle = (E_{\bar{N}}^0 + E_{\bar{N}}^0)/2$

Of course, if identical for all β as $\beta\to\infty$, $\langle\hat{N}\rangle = \bar{N} + 1/2$ But $\rightarrow$

Say $d_{\bar N} = d_{\bar N}^{\beta=\infty} + \frac{1}{\beta} a_{\bar N}$, $d_{\bar N+1} = d^{\infty}_{\bar N+1} + a_{\bar N+1} \cdot \frac{1}{\beta}$ & $d^{\infty}_{\bar N} = d^{\infty}_{\bar N+1}$

then $\beta d_{\bar N} = \beta d^{\infty}_{\bar N} + \bar a_N$, $\beta d_{\bar N+1} = \beta d^{\infty}_{\bar N+1} + a_{\bar N+1}$

so
$$\hat T = \frac{|\bar N\rangle\langle \bar N| \exp\left(-\beta d^{\infty}_{\bar N} - a_{\bar N}\right) + |\bar N+1\rangle\langle\bar N+1| \exp\left(-\beta d^{\infty}_{\bar N+1} - a_{\bar N+1}\right)}{\exp\left(-\beta d^{\infty}_{\bar N} - a_{\bar N}\right) + \exp\left(-\beta d^{\infty}_{\bar N+1} - a_{\bar N+1}\right)}$$

$$w_{\bar N} \equiv \frac{e^{-a_{\bar N}}}{e^{-a_{\bar N}} + e^{-a_{\bar N+1}}}, \quad w_{\bar N+1} = \frac{e^{-a_{\bar N+1}}}{e^{-a_{\bar N}} + e^{-a_{\bar N+1}}}, \quad w_{\bar N} + w_{\bar N+1} = 1$$

Then
$$\lim_{\beta\to\infty} \hat T = w_{\bar N} |\bar N\rangle\langle\bar N| + w_{\bar N+1} |\bar N+1\rangle\langle \bar N+1|$$

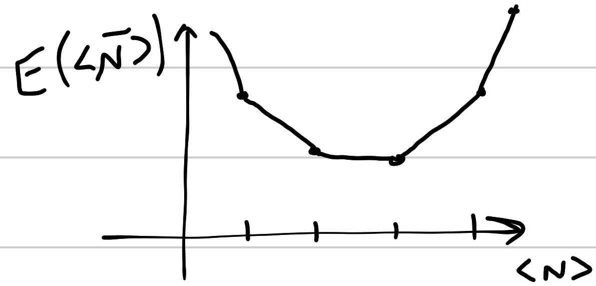
$$\langle \hat N\rangle = w_{\bar N}\cdot \bar N + (1-w_{\bar N})(\bar N+1)$$
$$\langle \hat H\rangle = w_{\bar N}\cdot E^{0}_{\bar N} + (1-w_{\bar N}) E^{0}_{\bar N+1}$$

Case ③ w/ ≥ 2 equal minima not possible due to concavity of E^{0}_{N}'

So if we let $\langle N\rangle = M+\delta$ M = integer, $0\leq\delta<1$

then $\langle \hat H\rangle = E^{0}_{M}\cdot(1-\delta) + E^{0}_{M+1}\cdot\delta$

series of line segments



A different proof is more about linear optimization

For $T=0$, only ground-states will contribute.

Let weights be ω_N where $0 \leq \omega_N \leq 1$

$$\& \quad \sum_N \omega_N = 1$$

$$\hat{T} = \sum_N |N\rangle\langle N| \cdot \omega_N$$

$$\langle \hat{H} \rangle = \sum_N \omega_N E_N \qquad \langle \hat{N} \rangle = \sum_N \omega_N N$$

Want to minimize $\langle \hat{H} \rangle$ over $\{\omega_N\}$ for fixed $\langle \hat{N} \rangle = M + \delta$ & $\sum_N \omega_N = 1$ & $0 \leq \omega_N \leq 1$.

So
$$\mathcal{F} \equiv \langle \hat{H} \rangle - \mu \langle \hat{N} \rangle - \alpha \sum_N \omega_N$$
$$= \sum_N (E_N - \mu N - \alpha)\omega_N$$

μ & α enforce the constraints so we freely minimize over $\{\omega_N\}$ & only need to worry about $0 \leq \omega_N \leq 1$.

$$\frac{\partial \mathcal{F}}{\partial \omega_N} = E_N - \mu N - \alpha = d_N$$

$$\delta \mathcal{F} = \sum_n d_N \cdot \delta\omega_N$$

At minimum: if $d_N = 0$, $\delta\omega_N$ unconstrained so $0 < \omega_N < 1$

if $d_N > 0$, $\omega_N = 0$ & $\delta\omega_N > 0$

if $d_N < 0$, $\omega_N = 1$ & $\delta\omega_N < 0$

$$d_N = E_N - (\overbrace{\mu N + \alpha}^{\text{straight line}})$$ & since E_N is concave up, only a finite # of $d_N \le 0$ is possible.

Case 1 some $d_M < 0$. So $\omega_M = 1$ & all $\omega_N = 0$ for $M \ne N$.

$\therefore$ pure state $\langle \hat{n} \rangle = M$, $\delta = 0$, $\langle \hat{\mathcal{H}} \rangle = E_M$

Case 2 minimum value of all $\{d_N\}$ is zero. If only a single one does this, back to case 1. If two, must be consecutive due to concavity. So only nonzero ω_N are ω_M & ω_{M+1}. $\omega_M + \omega_{M+1} = 1$ so $\omega_{M+1} \equiv \delta$

& $\langle \hat{n} \rangle = M + \delta$, $\langle \hat{\mathcal{H}} \rangle = E_M \cdot (1-\delta) + E_{M+1} \cdot \delta$

→ Can't have more than 2 $d_N = 0$ due to concavity

→ Can't have all $d_N > 0$ otherwise all $\omega_N = 0$?!?

So these two cases are all that can happen. Again, piecewise linear.

Why is E_N concave up?
- This argument requires it to be to give converging Z & $\hat{\Gamma}$ at finite β.
- Repulsive interactions generally make $E_{N+1} > E_N$ & more than linear
- Fermions, even non-interacting, must fill higher energy states as $N\uparrow$, so $\mu\uparrow$ & E_N concave up.