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 formalism:

$$\hat{\Gamma} = \frac{\exp(-\beta (\hat{H} - \mu \hat{N}))}{Z}$$

Let $Z = e^{\langle \hat{\theta} \rangle} = \text{tr}(\hat{\theta})$

$$\langle \hat{\theta} \rangle = \sum \sum |N_s><N_s| \exp(-\beta (E_s^0 - \mu \hat{N} - \alpha))$$

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

$$\hat{\Gamma} \to \sum_{N} |N_0><N_0| \exp(-\beta (E_0^0 - \mu N - \alpha))$$

Now consider $d_N = E_N^0 - \mu N - \omega$. As a function of $N$, $d_N$ must have a minimum value otherwise the sum won't converge. This means $E_0^0$ must be concave-up as a function of $N$ (since $\mu + \omega$ can take on various values).

**Case 1:** single minimum of $d_N$

For $N = N_\ast$,

then\thline (by the constraint $\sum_{N_0 < N_0} = 0$)
\begin{align*}
\langle \hat{N} \rangle &= N = \text{integer} \\
\langle \hat{\theta} \rangle &= E_0^0
\end{align*}

**Case 2:** two equal & consecutive minima for $N \& N+1$, \begin{align*}
\langle \hat{N} \rangle &= (N^0 + N^\ast)/2 \\
\langle \hat{\theta} \rangle &= (E_0^0 + E_N^0)/2
\end{align*}

Graphical construction is to draw line $MN + \omega$, $d_N$ is how far $E_0^0$ is above line.

Of course, if identical for all $\beta$ as $\beta \to \infty$, \begin{align*}
\langle \hat{N} \rangle &= N + 1/2 \\
\text{But} \to
\end{align*}
Let \( d_N = d_{-N}^\infty + \frac{1}{\beta} a_N \), \( d_{N+1} = d_{-N+1}^\infty + a_{N+1} \cdot \frac{1}{\beta} \) and \( d_N = d_{N+1}^\infty \)

then \( \beta d_N = \beta d_{-N}^\infty + a_N \), \( \beta d_{N+1} = \beta d_{-N+1}^\infty + a_{N+1} \)

As \( \gamma = \frac{\langle \bar{N} \rangle < \bar{N} | \exp (\beta d_{-N}^\infty - a_N) + | \bar{N}+1 \rangle < \bar{N}+1 | \exp (\beta d_{-N+1}^\infty - a_{N+1}) }{\exp (-\beta d_{-N}^\infty - a_N) + \exp (-\beta d_{-N+1}^\infty - a_{N+1})} \)

\( w_N = \frac{\exp (-a_N)}{\exp (-a_N - a_{N+1})} \), \( w_{N+1} = \frac{\exp (-a_{N+1})}{\exp (-a_{N+1} - a_N)} \), \( w_N + w_{N+1} = 1 \)

Then \( \lim_{\beta \to \infty} \gamma = w_N \langle \bar{N} \rangle < \bar{N} | + w_{N+1} \langle \bar{N}+1 \rangle < \bar{N}+1 | \)

\( \langle \bar{N} \rangle = w_N \bar{N} + (1-w_N) (\bar{N}+1) \)

\( \langle \bar{N} \rangle = w_N \cdot E_N^\circ + (1-w_N) E_{N+1}^\circ \)

Case 3: \( N \geq 2 \) equal minima not possible due to concavity of \( E_N \).

So if we let \( \langle N \rangle = M + \delta \) \( M = \text{integer}, \ 0 \leq \delta < 1 \)

then \( \langle \bar{N} \rangle = E_m^\circ \cdot (1-\delta) + E_{m+1}^\circ \cdot \delta \)

series of line segments \( E(\langle \bar{N} \rangle) \uparrow \)

\( \downarrow \) \( \langle \bar{N} \rangle \)
A different proof is more about linear optimization.

For \( t = 0 \), only ground-state will contribute.
Let weights be \( w_N \) where \( 0 \leq w_N \leq 1 \)
\[ \sum w_N = 1 \]
\[ \hat{\mathbf{P}} = \sum_{N} |N\rangle \langle N| \cdot w_N \]
\[ \langle \hat{\mathbf{P}} \rangle = \sum_{N} w_N E_N \]
\[ \langle N \rangle = \frac{\sum w_N N}{\sum w_N} \]

Want to minimize \( \langle \hat{\mathbf{P}} \rangle \) over \( \{w_N\} \) for fixed \( \langle \hat{N} \rangle = N + \delta \) and \( \sum w_N = 1 \) \( 0 \leq w_N \leq 1 \).

So
\[
\begin{align*}
F &= \langle \hat{\mathbf{P}} \rangle - \mu \langle \hat{N} \rangle - \alpha \sum w_N \\
&= \sum_{N} (E_N - \mu N - \alpha) w_N \\
\end{align*}
\]

\( \mu, \alpha \) enforce the constraints so we freely minimize over \( \{w_N\} \) but only need to worry about \( 0 \leq w_N \leq 1 \).

\[
\frac{\partial F}{\partial w_N} = E_N - \mu N - \alpha = d_N
\]
\[
\delta F = \sum_{N} d_N \cdot \delta w_N
\]

At minimum: if \( d_N = 0 \), \( \delta w_N \) unconstrained
\[
\begin{align*}
& \text{if } d_N > 0, \quad w_N = 0 \quad \delta w_N > 0 \\
& \text{if } d_N < 0, \quad w_N = 1 \quad \delta w_N < 0
\end{align*}
\]
\[ d_N = E_N - (\mu_N + \lambda) \] 

since \( E_N \) is concave up, only a finite # of \( d_N \leq 0 \) is possible.

Case 1: some \( d_M < 0 \). So \( \omega_M > 1 \) and \( \omega_N = 0 \) for \( M+N_0 \).

- pure state \( \langle \hat{n} \rangle = M, \quad s = 0 \), \( \langle \hat{\tau} \rangle = E_M \)

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 \( \omega_M = \omega_M + \omega_{M+1} \). \( \omega_M + \omega_{M+1} = 1 \rightarrow \omega_{M+1} = s \)

- \( \langle \hat{n} \rangle = M + s \), \( \langle \hat{\tau} \rangle = E_M (1-s) + E_{M+1} s \)

\[ \rightarrow \text{Can't have more than 2 } d_N = 0 \text{ due to concavity} \]

\[ \rightarrow \text{Can't have all } d_N > 0 \text{ otherwise all } \omega_n = 0 ?? \]

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 \( Z \) to \( \hat{n} \) at finite \( \beta \).
- Repulsive interactions generally make \( E_{N+1} > E_N \) more than linear
- Fermions, even non-interacting, must fill high energy states as \( N \rightarrow \infty \) and \( E_N \) concave up.