Idempotency of Density Matrix

Density matrix

\[ \hat{\rho} = \sum_m \frac{1}{\exp[\beta(E_m - \mu)] + 1} |m\rangle \langle m| \]  

(1)

where \( |m\rangle \) is an orthonormal basis set with energy eigenvalues \( E_m \).

[1] Normalization: Chemical potential equilibration

\[ f(\epsilon) = \frac{1}{\exp[\beta(\epsilon - \mu)] + 1} \]  

(2)

in the energy space, so as to satisfy the normalization to give the correct number of electrons \( N \).

\[ N = 2 \sum_m \frac{1}{\exp[\beta(E_m - \mu)] + 1} \]  

or

\[ N = \text{Tr} \hat{\rho} \]  

(3)

(4)
Idempotency: Pauli exclusion

\[ f(\epsilon) - f^2(\epsilon) = f(\epsilon)[1-f(\epsilon)] = f(\epsilon)\bar{f}(\epsilon) \geq 0 \]  

(4)

where \( \bar{f}(\epsilon) = 1 - f(\epsilon) \) is the unoccupation function. \( f-f^2 = \bar{f}f \) is thus the probability that the energy is both occupied & unoccupied. This is only nonzero within the small energy range near the chemical potential \( \mu \).

At zero temperature, \( f(\epsilon) - f^2(\epsilon) = 0 \) for \( \forall \epsilon \).

\[ \hat{\rho} - \hat{\rho}^2 = \sum_m |m\rangle f(\epsilon_m) \langle m| - \sum_m |m\rangle f(\epsilon_m) \langle m| - \sum_n |n\rangle f(\epsilon_n) \langle n| \]

\[ = \sum_m |m\rangle f(\epsilon_m) \langle m| - \sum_m |m\rangle f(\epsilon_m) \langle m| - \sum_n |n\rangle f(\epsilon_n) \langle n| \]

\[ = \sum_m |m\rangle \left[ f(\epsilon_m) - f^2(\epsilon_m) \right] \langle m| \]

\[ \therefore \hat{\rho} - \hat{\rho}^2 = \sum_m |m\rangle f(\epsilon_m) \left[ f(\epsilon_m) - f^2(\epsilon_m) \right] \langle m| \]

\[ \to 0 \quad (T \to 0) \]  

(6)
**Constraints on density matrix**

At zero-temperature,

1. **Normalization:** chemical potential equilibration
   \[
   \text{Tr} \hat{\rho} = N
   \]  
2. **Idempotency:** Pauli exclusion (or Fermi projection)
   \[
   \hat{\rho} - \hat{\rho}^2 = 0 \quad (\text{at } T=0)
   \]

The density matrix is thus obtained by

\[
\min \text{Tr} \hat{\rho} \hat{H} \text{ with constraints } \begin{cases} \text{Tr} \hat{\rho} = N & \text{Normalization:} \\ \hat{\rho} - \hat{\rho}^2 = 0 & \text{Idempotency:} \end{cases}
\]

If we explicitly introduce the Fermi filter \( f(\epsilon) \) in the density matrix as

\[
\hat{\rho} = \sum \text{Im} \langle m | f(\epsilon_m) | m \rangle
\]

then both normalization & idempotency constraints are built in.