Idempotency of Density Matrix

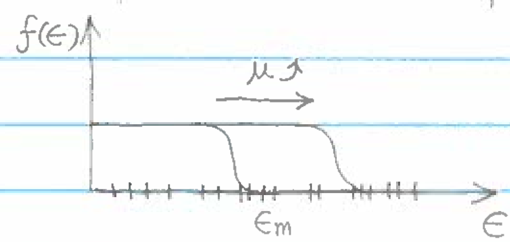
6/5/03

— Density matrix

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

where $\{|m\rangle\}$ is an orthonormal basis set with energy eigenvalues $\{\epsilon_m\}$.

[1] Normalization: Chemical potential equilibration



The chemical potential μ translates

$$f(\epsilon) = \frac{1}{\exp[\beta(\epsilon-\mu)]+1} \qquad (2)$$

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

$$N = 2\sum_m \frac{1}{\exp[\beta(\epsilon-\mu)]+1} \qquad (3)$$

or

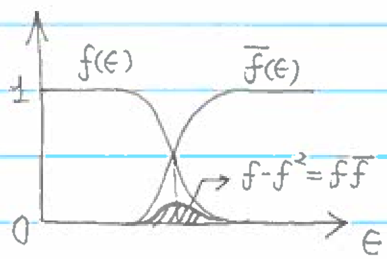
$$N = \mathrm{Tr}\,\hat{\rho} \qquad (4)$$

[2] Idempotency : Pauli exclusion

Note

$$f(\epsilon) - f^2(\epsilon) = f(\epsilon)[1 - f(\epsilon)] = f(\epsilon)\bar{f}(\epsilon) \geq 0 \qquad (4)$$

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



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

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

$$= \sum_m |m\rangle f(\epsilon_m) \langle m| - \underbrace{\sum_{m,n} |m\rangle f(\epsilon_m) \underbrace{\langle m|n\rangle}_{\delta_{mn}} f(\epsilon_n) \langle n|}_{\sum_m |m\rangle f^2(\epsilon_m) \langle m|}$$

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

$$\therefore \hat{\rho} - \hat{\rho}^2 = \sum_m |m\rangle f(\epsilon_m)[1 - f(\epsilon_m)] \langle m| \qquad (5)$$

$$\to \emptyset \quad (T \to 0) \qquad (6)$$

— Constraints on density matrix

At zero-temperature,

[1] Normalization: chemical potential equilibration

$$\mathrm{Tr}\,\hat{\rho} = N \tag{4}$$

[2] Idempotency: Pauli exclusion (or Fermi projection)

$$\hat{\rho} - \hat{\rho}^2 = 0 \quad (\text{at } T = 0) \tag{6}$$

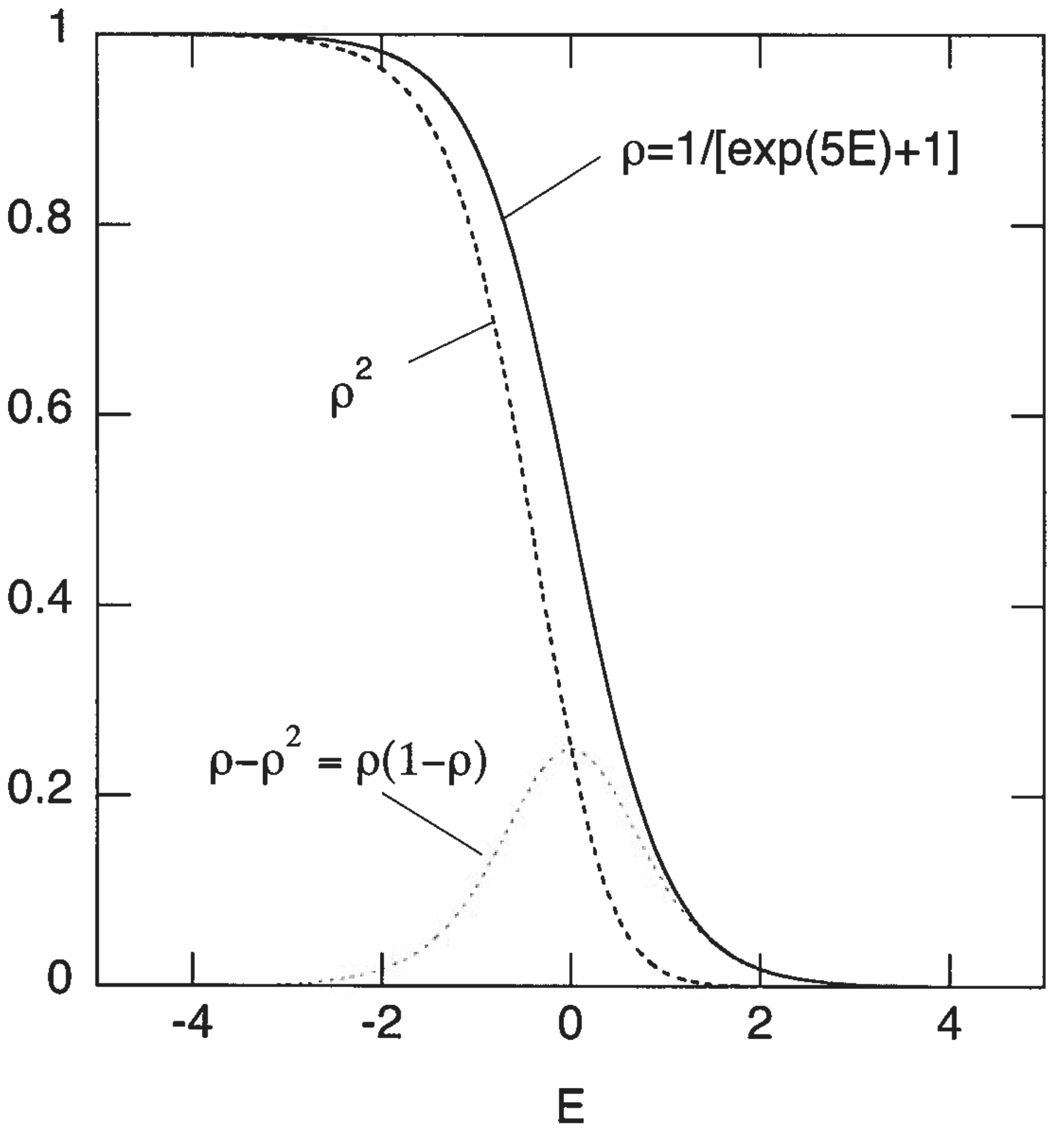
The density matrix is thus obtained by

$$\boxed{\min \mathrm{Tr}\,\hat{\rho}\hat{H} \quad \text{with constraints} \quad \underbrace{\mathrm{Tr}\,\hat{\rho} = N}_{\substack{\text{Normalization:}\\ \text{chemical}\\ \text{potential}\\ \text{equalization}}} \ \ \& \ \ \underbrace{\hat{\rho} - \hat{\rho}^2 = 0}_{\substack{\text{Idempotency:}\\ \text{Pauli}\\ \text{exclusion}}}} \tag{7}$$

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

$$\hat{\rho} = \sum_m |m\rangle f(\epsilon_m) \langle m|$$

then both normalization & idempotency constraints are built in.



ρ=1/[exp(5E)+1]
ρ^2
ρ−ρ^2 = ρ(1−ρ)
1
0.8
0.6
0.4
0.2
0
-4
-2
0
2
4
E