Exercise 1 - Fermi-Dirac Distribution (3 points)

Consider the Fermi-Dirac distribution function

$$n_F(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \tag{1}$$

where $\beta = 1/k_B T$ and μ is the chemical potential. Let $\epsilon(\vec{k}) = \hbar^2 \vec{k}^2/2m$ and ϵ_F is the energy of the highest occupied state at $T = 0$.

- Plot the distribution as a function of energy for different temperatures: $T = 0$, $k_B T < \epsilon_F$, and $k_B T > \epsilon_F$;
- Plot also the evolution of the chemical potential with temperature for these various cases;
- Plot the *derivative* (with respect to the energy) of the Fermi-Dirac distribution, again as a function of energy, for different temperatures: $T = 0$ and $T \neq 0$;
- Discuss the symmetry properties of $\frac{\partial n_F}{\partial \epsilon}$, with respect to the Fermi energy ϵ_F;
- Show that for $k_B T > \epsilon_F$, and for energies above the chemical potential, the Fermi-Dirac distribution reduces to the classical, Boltzmann distribution

$$n_F(\epsilon) \propto e^{-\epsilon/k_B T} \tag{2}$$

- If the above statement is made true for *all* energies, where is the chemical potential located in this case?

Exercise 2 - 4-site tight-binding chain (3 points)

Consider a 1-dimensional tight-binding model with 4 sites and periodic boundary conditions. The eigenstates are approximated by a linear combination of atomic orbitals (LCAO)

$$\psi_{nk}(r) = \sum_{R_i} c_k(R_i)\, \varphi_n(r - R_i) \tag{3}$$

where $\varphi_n(r - R_i)$ is the n-th atomic orbital localized around R_i and their overlap is assumed to be small.

(a) Determine the coefficients $c_k(R_i)$, using the lattice periodicity and the normalization condition.

(b) We assume the orbitals to be s-orbitals ($n = 1$). Let the matrix elements of H with respect to $|i\rangle$, an s-orbital at site R_i, be $\langle i|H|j\rangle = E_0\, \delta_{i,j} - t\, \delta_{i,j\pm 1}$. Write down and discuss the four lowest energy one-particle Eigenstates of the system.

(c) Consider two spinless fermions occupying the system. Derive their groundstate wavefunction.

Solutions due on: 24 June, 2011