Exercise 1 - Fermi-Dirac Distribution

Consider the Fermi-Dirac distribution function
\[ n_F(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu)} + 1} \]  
where \( \beta = 1/k_B T \) and \( \mu \) is the chemical potential. Let \( \epsilon(\vec{k}) = \hbar^2 \vec{k}^2 / 2m \) and \( \epsilon_F \) 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 \( \epsilon_F \);
- 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
\[ n_F(\epsilon) \propto e^{-\epsilon/k_B T} \]  
- 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

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)
\[ \psi_{nk}(r) = \sum_{R_i} c_k(R_i) \varphi_n(r - R_i) \]  
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