ECE 595 (Numerical Simulations) - Homework 2

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Please write your programs in C/C++ or MATLAB

Due February 1, 2013 at 4:30 pm

1. Consider the following dielectric function:

$$\epsilon(\omega) = \epsilon_o + \frac{f * \omega_o^2}{\omega_o^2 - \omega^2 + i\Gamma\omega} \tag{1}$$

where $\epsilon_o = 8$, $f = 10$, $\omega_o = 0.5$, $\Gamma = 0.2$. Please write a program to find the following:

a. A zero value for the real part of ϵ (and corresponding ω) within the range $\omega \in [0, 0.6]$

b. The minimum and maximum value of the real part of ϵ (and corresponding ω) within the range $\omega \in [0, 1]$.

2. Consider the following Hamiltonian for an array of localized electronic orbitals:

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij\sigma} C_{i\sigma}^\dagger C_{j\sigma} + U \sum_i n_{i\downarrow} n_{i\uparrow} \tag{2}$$

Where $n_{i\sigma} = C_{i\sigma}^\dagger C_{i\sigma}$, and the $C_{i\sigma}^\dagger$ creation and $C_{i\sigma}$ annihilation operators are fermionic. This gives rise to the eigenproblem $\mathcal{H}\psi = E\psi$. For $N = 2$ lattice sites at half-filling (i.e., two electrons), the state vector can be represented as $\psi = \left[C_{0\uparrow}^\dagger C_{1\uparrow}^\dagger, C_{0\downarrow}^\dagger C_{0\uparrow}^\dagger, C_{0\downarrow}^\dagger C_{1\uparrow}^\dagger, C_{0\uparrow}^\dagger C_{1\downarrow}^\dagger, C_{1\uparrow}^\dagger C_{1\downarrow}^\dagger, C_{0\downarrow}^\dagger C_{1\downarrow}^\dagger\right]^T |0\rangle$. Please write a program to find the following:

a. What are the eigenvalues and eigenvectors of the system when $t_{ij\sigma} = 0$, $U = 1$, and $N = 2$?

b. What are the eigenvalues and eigenvectors of the system,
when $U = 1$, $N = 2$, and $t_{ij\sigma} = \begin{cases} 1, & |i-j| = 1 \\ 0, & \text{otherwise} \end{cases}$?