Quantum Theory of Condensed Matter I

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Sheet 11

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1. Density of states for tight binding models (analytics)

Consider the following tight binding Hamiltonian representing the valence electrons of an infinite chain of atoms at distance a:

$$H = \lim_{N \to \infty} -t \sum_{i=1}^{N} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) \tag{1}$$

where for simplicity spin is neglected and we assume periodic boundary conditions.

1. Diagonalize the Hamiltonian.

(2 Points)

2. Prove that the density of states for the system reads (in the limit $N \to \infty$):

$$\rho(E) = \frac{1}{\pi} \frac{1}{\sqrt{4t^2 - E^2}}$$

for $|E| < 2t$ and vanishes elsewhere.

Hint: Start from the definition of the density of states:

$$\rho(E) = \frac{1}{N} \sum_\alpha \delta(E - E_\alpha)$$

where N is the total number of states for the system and α is labelling the eigenstates of the system with eigenvalue E_α. The following relation involving the Dirac distribution function can be useful:

$$\delta(f(x)) = \sum_i \frac{1}{|f'(x_i)|} \delta(x - x_i)$$

where x_i are all the points such that $f(x_i) = 0$

(2 Points)

3. What is the density of states for a 1-dimensional free electron gas? What does it have in common with the result calculated at point 1.2 ?

(2 Points)

2. Density of states of an infinite chain (numerics)

The density of states of a system can be calculated with the help of the Green's functions using the formula:

$$\rho(E) = \frac{1}{2\pi} \text{Tr}\{-2\text{Im}[G^r(E)]\}$$

where $G^r(E)$ is the retarded Green's function for the system defined as $G^r(E) = (E - H + i\eta)^{-1}$.

1. Construct numerically the Hamiltonian (1) given in the first exercise for a finite number of atoms $N = 2, 20, 200$ and, using the definition given above, calculate the corresponding Green's function. *Hint:* Values of η in the order of $\frac{2t}{N}$ are a good compromise between the requirement of small η and the energy grid necessary to resolve the structure of the Green's function.

(2 Points)

2. Starting from the Green's function calculated at the previous point, calculate the density of states normalized to the chain length $\tilde{\rho}(E) \equiv \frac{\rho(E)}{aN}$ where a is the distance between the atoms and compare the result with the analytical one obtained in the first exercise. *Hint:* Remember that the trace of a matrix is invariant under change of basis. The efficiency of the numerical calculation is in this case enormously enhanced in the eigenstates basis.

(2 Points)

Frohes Schaffen!