University of Regensburg Summer Term 2014

Quantum Theory of Condensed Matter I

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5.1.01 Mondays 10:15
9.2.01 Tuesdays 12:15

Sheet 5

1. Density of states for tight binding models

Consider the following tight-binding Hamiltonian representing the valence electrons of an infinite chain of atoms with the lattice constant a:

$$\hat{H} = \lim_{N_{\text{sites}}\to\infty} \left\{ -t \sum_{i=1}^{N_{\text{sites}}} (\hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_{i+1}^\dagger \hat{c}_i) \right\},$$

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

1. What is the first quantization Hamiltonian for this system? **(1 Point)**
2. Prove that the density of states for the system reads (in the limit $N_{\text{sites}} \to \infty$)

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

for $|E| < 2t$ and vanishes elsewhere. Hint: start from the definition of the density of states,

$$\rho(E) = \frac{1}{N_{\text{tot}}} \sum_\alpha \delta(E - E_\alpha),$$

where N_{tot} 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 delta can be useful:

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

where the points x_i are the zeroes of $f(x)$. **(2 points)**

3. What is the density of states for a 1-dimensional free electron gas? Compare it with the result calculated in the previous point. **(2 points)**

4. Now consider the generalization of the tight-binding model of an infinite chain to a square (2D) and a cubic (3D) lattice. What are the dispersion relations in these two cases? **(1 point)**

5. **(Oral)** Prove that the density of states can be reduced to the generic form

$$\rho_d(E) = \frac{1}{\pi} \int_0^\infty d\lambda\ \cos(\lambda E)\ J_0^d(2t\lambda),$$

where $J_0(x)$ is a Bessel function defined as

$$J_0(x) = \frac{1}{\pi} \int_0^\pi dy\ \exp(-ix\ \cos y)$$

and d is the dimensionality, $d = 1, 2, 3$. Hint: the following relations may be useful

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy\, e^{-ixy},$$
$$J_0(-x) = J_0^*(x) = J_0(x).$$

2. Occupation number representation

Let us consider a fermionic system with two single particle states $|\alpha\rangle$ and $|\beta\rangle$ that span the (two-dimensional) *one*-particle Hilbert space.

1. What is the dimension of the *two*-particle Hilbert space? What is the dimension of the Fock space? Write down the basis of the Fock space explicitly as Slater determinants of the wave functions $\phi_\alpha(\mathbf{r}), \phi_\beta(\mathbf{r})$ and in the occupation number representation. **(2 Points)**
2. Calculate, in the Fock basis, the matrix representation of the creation and annihilation operators $\hat{c}_\mu, \hat{c}_\mu^\dagger$ ($\mu = \alpha, \beta$) and also of the occupation operators $\hat{n}_\mu = \hat{c}_\mu^\dagger \hat{c}_\mu$. **(2 Points)**
3. Using explicitly the matrix multiplication of the matrices calculated in (b), calculate the anticommutator relations
$$[\hat{c}_\mu, \hat{c}_\nu]_+ = \left[\hat{c}_\mu^\dagger, \hat{c}_\nu^\dagger\right]_+ = 0; \qquad \left[\hat{c}_\mu, \hat{c}_\nu^\dagger\right]_+ = \delta_{\mu\nu}$$
(2 Points)

Frohes Schaffen!