PROBLEM SHEET 6

Introduction to Condensed Matter Theory

(To be submitted on Wednesday, 15.07.2015)

1. Tight-Binding Model on a Square Lattice: Consider a tight-binding model on a two-dimensional square lattice (lattice spacing a) with on-site energy ε^0 and nearest-neighbour hopping matrix element t:

$$H = \sum_{\mathbf{r}} \{\varepsilon^0 |\mathbf{r}\rangle\langle\mathbf{r}| + t[|\mathbf{r}\rangle\langle\mathbf{r}+a\hat{x}| + |\mathbf{r}\rangle\langle\mathbf{r}-a\hat{x}| + |\mathbf{r}\rangle\langle\mathbf{r}+a\hat{y}| + |\mathbf{r}\rangle\langle\mathbf{r}-a\hat{y}|]\} \tag{1}$$

(a) Obtain the dispersion relation for this model and plot it for the first Brillouin zone. (*Try to obtain the plot numerically if possible*) [3]

(b) Plot the Fermi surface in the first Brillouin zone for the following cases with explanation: (i) less than a half-filled band (ii) exactly half-filled band (iii)more than half-filled band. In which cases will the material be an insulator or a metal? [3+1]

(c) Calculate the density of states for this case of a square lattice (*Or write a piece of code to obtain it numerically*). Obtain the plot. Also, explain how does the plot look like for the case of $d = 1$ and $d = 3$(for a cubic lattice). [2+1+1]

2. Second Quantization: In the formalism of second quantization, a general state of N particles at positions $\vec{r}_1, \vec{r}_2$...is given by

$$|\vec{r}_1, \vec{r}_2, ..., \vec{r}_N\rangle = \frac{1}{\sqrt{N!}} \hat{\Psi}^\dagger(r_N)...\hat{\Psi}^\dagger(r_1)|0\rangle \tag{2}$$

where $|0\rangle$ is the vacuum state and the field operators $\hat{\Psi}(\vec{r})$ are defined as

$$\hat{\Psi}(\vec{r}) = \sum_k \phi_k(\vec{r})\hat{a}_k \tag{3}$$

with $\hat{a}_k$ the annihilator of mode k and $\phi_k(\vec{r})$ the one particle wave function of mode k.
(a) Consider a state $|\psi\rangle$ of three particles in modes k_1, k_2 and k_3. Consider its wavefunction

$$\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \langle\vec{r}_1, \vec{r}_2, \vec{r}_3|\psi\rangle = \langle\vec{r}_1, \vec{r}_2, \vec{r}_3|\hat{a}^\dagger_{k_3}\hat{a}^\dagger_{k_2}\hat{a}^\dagger_{k_1}|0\rangle. \tag{4}$$

Calculate the vacuum expectation value

$$\langle 0|\hat{a}_{l_1}\hat{a}_{l_2}\hat{a}_{l_3}\hat{a}^\dagger_{k_3}\hat{a}^\dagger_{k_2}\hat{a}^\dagger_{k_1}|0\rangle, \tag{5}$$

for bosons and for fermions. [2]

(b) Determine $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ for bosons and for fermions. What symmetries does the wavefunctions possess? [2]

(c) Determine the normalization of the wavefunction for fermions and for bosons. First consider the case where k_1, k_2 and k_3 are all different, and then study the case where two or more modes are the same. What do you observe? [2+2+1]

—- Keep Calm and Good Luck for the Exams —-