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 6

1. The Hubbard model

The Hamiltonian of a system of N electrons is given by

$$\hat{H} = \hat{T}_e + \hat{V}_{ie} + \hat{V}_{ee} = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i=1}^{N} V(\mathbf{r}_i) + \sum_{i \neq j} \frac{e^2}{\mathbf{r}_i - \mathbf{r}_j},$$

where $\hat{T}_e$ is the kinetic energy of the electrons, $\hat{V}_{ie}$ is the periodic potential generated by the ions and $\hat{V}_{ee}$ is the Coulomb potential defining the electron-electron interaction.

1. Express this Hamiltonian in the second quantization, both in the Wannier and the Bloch basis. Assume that there is only one band, so the only quantum numbers are the spin σ, and $\mathbf{k}$ or $\mathbf{R}$ depending on the basis. **(2 Points)**
2. Use the tight-binding approximation assuming only the nearest-neighbour hopping and write down the matrix elements of $\hat{V}_{ee}$ in the Wannier basis. **(2 Points)**
3. The tight-binding, nearest-neighbour approximation implies that only 5 terms in the sums over $\mathbf{r}$'s are non-vanishing. The most significant are the on-site interaction U and the nearest-neighbour interaction V. What are the matrix elements corresponding to these two terms, in the Wannier basis? **(2 Points)**
4. Prove that if only the single-electron part and the on-site part of the Coulomb interaction are taken into account, the Hubbard hamiltonian can be written as

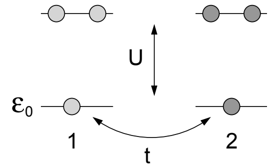
$$H = \sum_{\mathbf{R},\mathbf{R}'(\text{n.n.})} \sum_{\sigma} t c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}'\sigma} + U \sum_{\mathbf{R}} c^{\dagger}_{\mathbf{R}\uparrow} c_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}\downarrow} c_{\mathbf{R}\downarrow}.$$

(2 Points)

2. Double site Hubbard model

The Hubbard Hamiltonian for a two site system reads explicitly:

$$\begin{aligned}\hat{H} &= \epsilon_0 \left(\hat{c}^{\dagger}_{1\uparrow}\hat{c}_{1\uparrow} + \hat{c}^{\dagger}_{1\downarrow}\hat{c}_{1\downarrow} + \hat{c}^{\dagger}_{2\uparrow}\hat{c}_{2\uparrow} + \hat{c}^{\dagger}_{2\downarrow}\hat{c}_{2\downarrow} \right) + t \left(\hat{c}^{\dagger}_{1\uparrow}\hat{c}_{2\uparrow} + \hat{c}^{\dagger}_{2\downarrow}\hat{c}_{1\downarrow} + \hat{c}^{\dagger}_{2\uparrow}\hat{c}_{1\uparrow} + \hat{c}^{\dagger}_{1\downarrow}\hat{c}_{2\downarrow} \right) \\ &+ U \left(\hat{c}^{\dagger}_{1\uparrow}\hat{c}_{1\uparrow}\hat{c}^{\dagger}_{1\downarrow}\hat{c}_{1\downarrow} + \hat{c}^{\dagger}_{2\uparrow}\hat{c}_{2\uparrow}\hat{c}^{\dagger}_{2\downarrow}\hat{c}_{2\downarrow} \right).\end{aligned}$$



1. Calculate the two particle eigenenergies analytically. Treat the case of parallel and antiparallel spin separately. Assume a fixed $t < 0$ and plot the results as a function of U/t.
   Hint: For the antiparallel case consider the basis of the corresponding Hilbert space:
   $$\hat{c}^{\dagger}_{1\uparrow}\hat{c}^{\dagger}_{1\downarrow}|0\rangle, \quad \hat{c}^{\dagger}_{2\uparrow}\hat{c}^{\dagger}_{2\downarrow}|0\rangle, \quad \hat{c}^{\dagger}_{1\uparrow}\hat{c}^{\dagger}_{2\downarrow}|0\rangle, \quad \hat{c}^{\dagger}_{2\uparrow}\hat{c}^{\dagger}_{1\downarrow}|0\rangle.$$
   Calculate the matrix elements of $\hat{H}$ in this basis and diagonalize the resulting 4×4 matrix. **(3 Points)**
2. **(Oral)** Calculate the ground state in the Hartree-Fock approximation and compare it with the exact result from 2.1.

Frohes Schaffen!