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Condensed Matter Field Theory — WS09/10

Exercise 1

(Please return your solutions before Fr. 30.10. 12:00h)

1.1. Operators in 2nd quantization (20 points)

We consider a system of N identical particles. The Hamiltonian is comprised of the kinetic energy $T = \sum_i \mathbf{p}_i/2m$, the single-particle potential $U(\mathbf{r})$ and a two-body interaction $V(\mathbf{r}_i, \mathbf{r}_j)$:

$$H = \sum_i \frac{\mathbf{p}_i}{2m} + U(\mathbf{r_i}) + \frac{1}{2}\sum_{i\neq j} V(\mathbf{r}_i, \mathbf{r}_j). \tag{1}$$

a) Show that the 2nd quantized form of (1), both for fermions and bosons is given by

$$H = \sum_{\alpha,\beta} (T_{\alpha\beta} + U_{\alpha\beta})\, a^\dagger_\alpha a_\beta + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha\beta\gamma\delta}\; a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma,$$

where $\{|\alpha\rangle\}$ is a complete and orthonormal single-particle basis. The matrix elements are given by

$$T_{\alpha\beta} = \langle\alpha|\, T\, |\beta\rangle$$
$$U_{\alpha\beta} = \langle\alpha|\, U\, |\beta\rangle$$

and

$$V_{\alpha\beta\gamma\delta} = \langle\alpha|\,\langle\beta|\, V\, |\gamma\rangle\, |\delta\rangle.$$

Remark: You only need to show this for the fermionic ***or*** *the bosonic case.*

b) Now consider as a single-particle basis the momentum eigenstates of free particles in a volume V,

$$\phi_\mathbf{k}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{kr}},$$

which fullfill the orthogonality relation:

$$\int d^3r \phi^*_\mathbf{k}(\mathbf{r})\phi_{\mathbf{k}'}(\mathbf{r}) = \delta_{\mathbf{kk}'}.$$

Assume translational invariance $V(\mathbf{r}_i, \mathbf{r}_j) = V(|\mathbf{r}_i - \mathbf{r}_j|)$ to show that the momentum representation of (1) reads

$$H = \sum_\mathbf{k} \frac{(\hbar\mathbf{k})^2}{2m} a^\dagger_\mathbf{k} a_\mathbf{k} + \frac{1}{V}\sum_{\mathbf{k},\mathbf{k}'} U_{\mathbf{k}-\mathbf{k}'} a^\dagger_{\mathbf{k}'} a_\mathbf{k} + \frac{1}{2V}\sum_{\mathbf{q},\mathbf{p},\mathbf{k}} V_\mathbf{q} a^\dagger_{\mathbf{p}+\mathbf{q}} a^\dagger_{\mathbf{k}-\mathbf{q}} a_\mathbf{k} a_\mathbf{p}$$

where $V_\mathbf{q}$ and $U_\mathbf{q}$ are the Fourier transform of the single-particle potential and the two-body interaction respectively.

1.2. Hubbard model (10 points)

We consider a system of non-interacting electrons ($V = 0$) in a periodic potential ($U(\mathbf{r}+\mathbf{R}) = U(\mathbf{r})$, $\mathbf{R} \in$ lattice).

$$H_0 = \sum_i \frac{\mathbf{p}_i}{2m} + U(\mathbf{r_i})$$

The eigenstates of this single-particle problem are Bloch modes:

$$H_0 \psi_{\mathbf{k}\sigma}(\mathbf{r}) = \epsilon(\mathbf{k}) \psi_{\mathbf{k}\sigma}(\mathbf{r})$$

where $\epsilon(\mathbf{k})$ defines the band structure. Since we consider a single band the band index was suppressed. Bloch functions can be written as:

$$\psi_{\mathbf{k}\sigma}(\mathbf{r}) = \langle \mathbf{r} | \mathbf{k}\sigma \rangle = u_{\mathbf{k}\sigma}(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} \chi_\sigma,$$

where $u_{\mathbf{k}\sigma}$ has the same symmetry as the lattice and $\mathbf{k} \in$ BZ (Brillouin zone). χ_σ describes the spin. Bloch functions are orthonormal:

$$\int d^3 r \psi^*_{\mathbf{k}\sigma}(\mathbf{r}) \psi_{\mathbf{k}'\sigma}(\mathbf{r}) = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}.$$

The Fourier transform of Bloch functions are called Wannier functions

$$w_{\mathbf{R}_i\sigma}(\mathbf{r}) = \langle \mathbf{r} | i\sigma \rangle = \frac{1}{\sqrt{N_l}} \sum_{\mathbf{k} \in \mathrm{BZ}} e^{-i\mathbf{k}\mathbf{R}_i} \psi_{\mathbf{k}\sigma}(\mathbf{r})$$

where N_l is the number of lattice points. Bloch functions are extended over the whole lattice. In contrast to that the Wannier function $w_{\mathbf{R}_i\sigma}$ is localized around $\mathbf{R}_i$.

a) Write down the H_0 in 2nd quantization in the basis of Bloch states.

b) Write down the H_0 in 2nd quantization in the basis of Wannier states.
Hint:

$$\sum_{\mathbf{k} \in \mathrm{BZ}} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} = N_l \delta_{ij}$$

Now we take the Coulomb interaction between the electrons into account. For a system with negligible interatomic overlap, i.e. the lattice potential approaches a superposition of atomic potentials, the Wannier function $w_{\mathbf{R}_i\sigma}(\mathbf{r})$ converge on the atomic orbital centered around $\mathbf{R}_i$. In this limit, one can neglect the overlap of two Wannier functions centered around different lattice sites.

c) Show that in this approximation the full Hamiltonian (1) is given in Wannier representation as

$$H = \sum_{ij\sigma} T_{ij} a^\dagger_{i\sigma} a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \tag{2}$$

where $n_{i\sigma} = a^\dagger_{i\sigma} a_{i\sigma}$ is the particle number operator. And the on-site repulsion is $U = V_{iiii}$. This is the famous *Hubbard model.*

d) Calculate (2) in Bloch representation. *Hint:* Write $a_{i\sigma}$ as a Fourier transform with respect to $\mathbf{k}$.