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Condensed Matter Theory I — WS09/10

Exercise 3

(Please return your solutions before Fr., 20.11., 12:00h)

3.1 Tight binding model (12 points)

We consider a d-dimensional cubic lattice ($d = 1, 2, 3$) with lattice constant a and a single atom on each lattice site $\mathbf{R}_i$. In contrast to exercise 2.2 where we have assumed a weak periodic potential as a perturbation of a free electron gas we will investigate the case of a strong periodic potential here. This leads to a limited electron mobility and an enhancement of the electron probability density around the lattice sites $\mathbf{R}_i$. By expanding the Bloch functions of a given band in terms of atomic orbitals and making use of the translation behavior and the orthogonality of Bloch functions one obtains

$$\psi_{\mathbf{k}}(\mathbf{r}) \approx \frac{1}{\sqrt{N}} \sum_i e^{\mathrm{i}\mathbf{k}\mathbf{R}_i} \phi_i(\mathbf{r}).$$

$\phi_i(\mathbf{r})$ is the atomic orbital centered around the lattice site $\mathbf{R}_i$. Since the interatomic overlap is assumed to be small one can neglect all integrals containing atomic orbitals which are separated by more than a lattice constant:

$$\langle \phi_i | H | \phi_j \rangle = \begin{cases} \epsilon_0 & , \quad i = j \\ -t_{ij} & , \quad i \text{ and } j \text{ nearest neighbors} \\ 0 & , \quad \text{else} \end{cases} ,$$

where t_{ij} is the so called *hopping* matrix elements since it describes the hopping of an electron from one lattice site to another. We assume isotropic atomic orbitals (s-waves) and set $t_{ij} = t$.

(a) Calculate the bandstructure $\epsilon(\mathbf{k})$ for $d = 1, 2, 3$.

(b) Sketch for the two dimensional case the lines of constant energy $\epsilon(\mathbf{k}) = \mathit{const.}$ in the 1st Brillouin zone. In particular, draw the constant energy lines in the band center, $\epsilon(\mathbf{k}) = \epsilon_0$.

(c) Determine the positions of the van Hove singularities by calculating the group velocity $v_{\mathbf{k}}$ for $d = 1, 2$. Calculate the density of states $N(\epsilon)$ for the one dimensional case.

(d) Show for $d = 2$ that the van Hove singularity at $\epsilon(\mathbf{k}) = \epsilon_0$ is logarithmically divergent.

Hint: Expand the group velocity around the saddle point $\kappa = (0, -\pi/a)$ up to second order. Afterwards evaluate $N(\epsilon = \epsilon_0 + \delta)$ for a small δ by approximating the corresponding curve of equal energy by a line, e.g. $k_x = k_y + \Delta k$.

(e)* Use a computer to plot $N(\epsilon)$ for $d = 2, 3$.
Hint: Use the formular:

$$N(\epsilon) = \sum_{\mathbf{k}} \delta_{\epsilon,\epsilon(\mathbf{k})}$$

3.2 The free electron Green's function (8 points)

The equation of motion for the free electron Green's function reads

$$(E - H_0)G(\mathbf{r} - \mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}') \tag{1}$$

with H_0 the kinetic energy operator. In the following we want to derive the expression for $G(\mathbf{r} - \mathbf{r}')$.

(a) Perform the Fourier transform of (1) to $\mathbf{k}$-space and solve the equation for $G_E(\mathbf{k})$.

(b) Derive by back-transforming to $\mathbf{r}$-space the solution $G(\mathbf{r})$ of (1).

(c) Use the same calculation for dimension $d = 1$ and derive $G(r)$.

3.3 The Green's function method for lattice electrons (KKR) (10 points)

The Schrödinger equation for the Bloch function $\Psi_{\mathbf{k}}$ is given by

$$(E - H_0)\Psi_{\mathbf{k}}(\mathbf{r}) = U(\mathbf{r})\Psi_{\mathbf{k}}(\mathbf{r}) \,.$$

with the kinetic energy H_0 and the crystal potential $U(\mathbf{r})$. The Green's function for the Schrödinger equation is defined by

$$(E - H_0)G(\mathbf{r} - \mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}') \,. \tag{2}$$

(a) Show that if $G_E(\mathbf{r} - \mathbf{r}')$ is a solution of equation (2) the wave function $\Psi_{\mathbf{k}}(\mathbf{r})$ is given by the following integral equation:

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \int d^3r' \, G_E(\mathbf{r} - \mathbf{r}')U(\mathbf{r}')\Psi(\mathbf{r}') \tag{3}$$

(b) Now, the crystal potential is given by $U(\mathbf{r}) = \sum_{\mathbf{R}} V(\mathbf{r} - \mathbf{R})$ with the lattice vector $\mathbf{R}$ and $V(\mathbf{r} - \mathbf{R})$ the potential of the atom at site $\mathbf{R}$. Plug this into the integral equation (3) and derive for the wave function:

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \int d^3r' \, \mathcal{G}_{\mathbf{k},E}(\mathbf{r} - \mathbf{r}')V(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}') \tag{4}$$

Herein,

$$\mathcal{G}_{\mathbf{k},E}(\mathbf{r} - \mathbf{r}') := \sum_{\mathbf{R}} e^{i\mathbf{k}\mathbf{R}} G_E(\mathbf{r} - \mathbf{r}' - \mathbf{R})$$

is the lattice Green's function.
The $\mathbf{k}$-dependence and the crystal structure completely pass into $\mathcal{G}_{\mathbf{k},E}(\mathbf{r} - \mathbf{r}')$.

$V(\mathbf{r}')$ is the atomic core potential with $V(\mathbf{r}') \neq 0$ only for $|\mathbf{r}'| < r_0$. Therefore, the integral in equation (4) extends only over the atomic core region.
This means for the calculation of the wave function that $\Psi_{\mathbf{k}}(\mathbf{r})$ can be derived for the complete space, once it is known for the atomic core region.
To obtain $\Psi_{\mathbf{k}}(\mathbf{r}')$ for $|\mathbf{r}'| < r_0$ the boundary conditions have to be fixed.

(c) Use the Schrödinger equation for $|\mathbf{r}'| < r_0$ and eliminate $V(\mathbf{r}')$ in (4). Show that

$$\int_{core} d^3r'\, \nabla' \left[\mathcal{G}_{\mathbf{k},E}(\mathbf{r}-\mathbf{r}')\nabla'\Psi_{\mathbf{k}}(\mathbf{r}') - \Psi_{\mathbf{k}}(\mathbf{r}')\nabla'\mathcal{G}_{\mathbf{k},E}(\mathbf{r}-\mathbf{r}')\right] = 0 \qquad (5)$$

is valid for all $\mathbf{r}$.
Hint: Use the fact that in the core region for $\mathcal{G}_{\mathbf{k},E}(\mathbf{r}-\mathbf{r}')$ the same relation holds as for the free electron Green's function (2).
In addition to this use the formula:

$$\nabla'[\mathcal{G}\nabla'\Psi - \Psi\nabla'\mathcal{G}] = \mathcal{G}\nabla'^2\Psi - \Psi\nabla'^2\mathcal{G}\,.$$

As a last step we can rewrite expression (5) using Gauss' theorem and derive a surface boundary condition. With this the wave function $\Psi_k(\mathbf{r})$ can be determined uniquely in the core region.