Quantum theory of condensed matter I

PD Dr. Andrea Donarini

Dr. Ivan Dmitriev

Tue	10:00 - 12:00	H33
Thu	10:00 - 12:00	H33
Tue	12:00 - 14:00	9.2.01

Sheet 2

1. Fourier transform of the Yukawa and Coulomb potential

The 3D Yukawa potential is given by $V_Y(\mathbf{r}) = r^{-1}e^{-\alpha r}$ $(\alpha > 0, r \equiv |\mathbf{r}|)$.
1. Calculate the Fourier transform $F_Y(\mathbf{k}) = \int d\mathbf{r} V_Y(\mathbf{r}) \exp(-i\mathbf{k}\cdot\mathbf{r})$ of the Yukawa potential **(3 Points)**
2. Find the Fourier transform $F_C(\mathbf{k})$ of the Coulomb potential $V_Y(\mathbf{r}) = 1/r$ **(1 Point)**.

2. Cubic Bravais lattices in the direct and reciprocal spaces

Prove that the body-centered and face-centered cubic (bcc and fcc) Bravais lattices are reciprocal to each other **(3 points)**.
As a warm-up, show that a simple cubic (sc) Bravais lattice is reciprocal to itself (in the sense that the reciprocal lattice is also an sc lattice) **(1 point)**.
Hint: Take the basis vectors in one of them and show explicitly that the corresponding basis in the reciprocal space coincides (as far as the symmetry is concerned) with the basis of the other. It is convenient to use a symmetric basis, for instance
sc: $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} = a\{(1,0,0),(0,1,0),(0,0,1)\}$
fcc: $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} = (a/2)\{(0,1,1),(1,0,1),(0,1,1)\}$
bcc: $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} = (a/2)(-1,1,1),(1,-1,1),(1,1,-1)$

3. Density of states in the reciprocal space (oral)

Consider an electron in a cubic region of free space with the volume L^3. In case (a), the boundary conditions require the electron wave function to be zero at the boundary of the region. In case (b), the boundary conditions are periodic (Bornvon Karman boundary conditions). Find the restrictions on the values of momentum the electron may have in both cases and calculate the density of states (the number of allowed momentum states per unit volume in the momentum space). Hint: the density of states should be the same in both cases!

Imagine that the cubic region is not a free space but a monocrystal. Which boundary conditions are compatible with the Bloch states? What other states may appear with different types of the boundary conditions?

4. *towards* Kramers theorem (oral)

Consider an homoatomic crystal structure $\mathbf{R}_\alpha$ which is invariant under the inversion operation $\mathcal{I} : \mathbf{r} \to -\mathbf{r}$ and under the rotation $R_{\phi,\mathbf{n}}$ about an angle ϕ around the direction fixed by the vector $\mathbf{n}$. Prove the following identities for the spectrum of the Bloch states:

$$\epsilon_\nu(\mathbf{k}) = \epsilon_\nu(\mathcal{I}\mathbf{k}) \qquad \text{and} \qquad \epsilon_\nu(\mathbf{k}) = \epsilon_\nu(\mathbf{R}_{\phi,\mathbf{n}}\mathbf{k}).$$

Hint: You could start from the equation (2.28) presented in the lecture giving the eigenvalues of the Bloch states and analyze how the symmetry operations of the crystal affects $\gamma(\mathbf{R})$.

Frohes Schaffen!