Quantum Theory of Condensed Matter

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Room H33
Wednesdays at 16:15

Sheet 12

1. Lattice dynamics of a square lattice

Consider a mono-atomic, two-dimensional square lattice of N^2 atoms of mass M with periodic boundary conditions and $N \to \infty$. The basis vectors are $\mathbf{a}_1 = a\hat{x}$ and $\mathbf{a}_2 = a\hat{y}$. Assume a potential energy for deformation with the form:

$$V = \frac{k}{2} \sum_{\langle i,j \rangle} \|\mathbf{u}_i - \mathbf{u}_j\|^2 \,,$$

where $\langle i,j \rangle$ denotes nearest neighbour lattice sites and $\mathbf{u_i}$ is the displacement of atom i from the equilibrium position $\mathbf{R_i^0}$.

1. Show that the force strength matrices $\tilde{\mathbf{D}}(\mathbf{R}_k^0)$ are diagonal and nonzero up to $\mathbf{R}_k^0 = \mathbf{0}$ or $\mathbf{R}_k^0 = \pm\mathbf{a}_1, \pm\mathbf{a}_2$. With a harmless abuse of notation we define, for the periodic lattice at hand, $\tilde{D}_{\alpha\beta}(\mathbf{R}_\ell^0, \mathbf{R}_m^0) = \tilde{D}_{\alpha\beta}(\mathbf{R}_\ell^0 - \mathbf{R}_m^0)$. Remember the definition of the force strength matrices and their sum rule:

$$\tilde{D}_{\alpha\beta}(\mathbf{R}_\ell^0, \mathbf{R}_m^0) = \left. \frac{\partial^2 V}{\partial u_\ell^{(\alpha)} \partial u_m^{(\beta)}} \right|_{\mathbf{u}_k \equiv 0,\ \forall k} ,$$

$$\sum_{k=1}^{N^2} \tilde{D}_{\alpha\beta}(\mathbf{R}_k^0) = 0.$$

   where α, β indicate the x or y component.

2. Write the equations of motion for the displacements and their associated momenta in terms of the force strength matrices by making use of the standard exponential Ansatz seen in class. The problem is transformed into the calculus of the 2×2 dynamical matrix

$$D_{\alpha\beta}(\mathbf{q}) = \sum_k \tilde{D}_{\alpha\beta}(\mathbf{R}_k^0) \exp\left(-i\mathbf{q} \cdot \mathbf{R}_k^0\right) .$$

3. The eigenvalues of $\mathbf{D}(\mathbf{q})$ are $M\omega_\lambda^2(\mathbf{q})$ with the two – in this case they are degenerate – phonon frequencies $\omega_\lambda(\mathbf{q})$. Plot the dispersion relation ω vs. $\mathbf{q}$ for the special directions of $\mathbf{q}$: $\Gamma \to \mathrm{X} \to \mathrm{M} \to \Gamma$. The high symmetry points Γ, X, M in the reciprocal space lattice are

$$\Gamma = (0,0) \,, \quad \mathrm{X} = \left(\frac{\pi}{a}, 0\right) , \quad \mathrm{M} = \left(\frac{\pi}{a}, \frac{\pi}{a}\right) .$$

Frohes Schaffen!