Quantum theory of condensed matter I

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

Sheet 6

1. Lattice dynamics of a square lattice

Consider a monoatomic, 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 $\mathbf{a}_2 = a\hat{y}$. The potential energy for deformation can be written in the form: $V = V_{\text{static}} + V_{\text{harm}} + O(u^4)$ where the harmonic component reads $V_{\text{harm}} = \frac{1}{2}\sum_{n,m}\sum_{\alpha\beta}(\vec{u}_\alpha)_n \Phi_{nm}(\vec{R}^0_\alpha - \vec{R}^0_\beta)(\vec{u}_\beta)_m$.

Assume now a harmonic component having the form:

$$V_{\text{harm}} = \frac{\kappa}{2}\sum_{\langle\alpha,\beta\rangle} |\vec{u}_\alpha - \vec{u}_\beta|^2 ,$$

where $\langle\alpha,\beta\rangle$ denotes nearest neighbor lattice sites and $\vec{u}_\alpha$ is the displacement from the equilibrium position $\vec{R}^0_\alpha$.

1. Show that the force strength matrices $\Phi(\vec{R}^0_\gamma)$ are diagonal and nonzero up to $\vec{R}^0_\gamma = \mathbf{0}$ or $\vec{R}^0_\gamma = \pm\mathbf{a}_1, \pm\mathbf{a}_2$. Remember the definition of the force strength matrices and their sum rule:

$$\begin{aligned} \Phi_{nm}(\vec{R}^0_\alpha - \vec{R}^0_\beta) &= \left.\frac{\partial^2 V}{\partial u^{(n)}_\alpha \partial u^{(m)}_\beta}\right|_{\vec{u}_\gamma = 0,\ \forall\gamma}, \\ \sum_{\gamma=1}^{N^2} \Phi_{nm}(\vec{R}^0_\gamma) &= 0. \end{aligned}$$

   where n, m indicate the x or y component. **(3 Points)**

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

$$\tilde{D}_{nm}(\vec{q}) = \frac{1}{M}\sum_\gamma \Phi_{nm}(\vec{R}^0_\gamma)\exp\left(-i\vec{q}\cdot\vec{R}^0_\gamma\right).$$

   (3 Points)

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

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

   (3 Points)

Frohes Schaffen!