Exploring Quantum Physics

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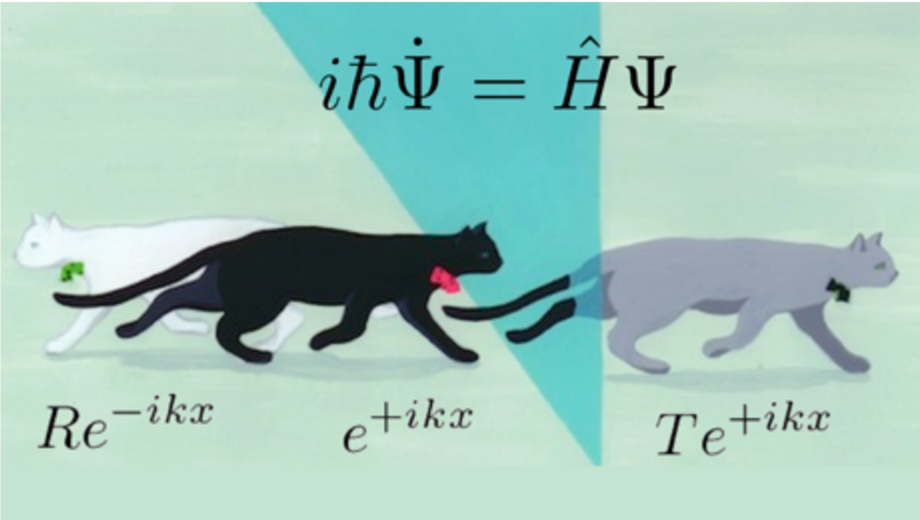
Phonons in crystals

Part IV: Bogoliubov transformation; quantum phonons



Where we've been and where we are going

$$H = \sum_n \left[\frac{p_n^2}{2m} + \frac{k}{2} \left(x_n - x_{n+1} \right)^2 \right]$$

$x_n, \, p_n$

Where we've been and where we are going

$$H = \sum_n \left[\frac{\hat{p}_n^2}{2m} + \frac{k}{2} \left(\hat{x}_n - \hat{x}_{n+1} \right)^2 \right]$$

$$x_n,\ p_n \longrightarrow \hat{x}_n,\ \hat{p}_n = -i\hbar \frac{\partial}{\partial x_n}$$

Where we've been and where we are going

$$\hat{H} = \frac{\hbar\omega}{4}\sum_n \left[-\left(\hat{a}_n^\dagger - \hat{a}_n\right)^2 + \left(\hat{a}_n^\dagger + \hat{a}_n - \hat{a}_{n+1}^\dagger + \hat{a}_{n+1}\right)^2\right]$$

$$x_n,\ p_n \longrightarrow \hat{x}_n,\ \hat{p}_n = -i\hbar\frac{\partial}{\partial x_n}$$

$$\downarrow$$

$$\hat{a}_n,\ \hat{a}_n^\dagger \text{ with } \left[\hat{a}_n,\ \hat{a}_m^\dagger\right] = \delta_{n,m}$$

Where we've been and where we are going

$$\hat{H} = \int_q \left[A(q)\hat{a}_q^\dagger \hat{a}_q + B(q)\hat{a}_q\hat{a}_{-q} + \text{H.c.}\right]$$

$$x_n,\, p_n \longrightarrow \hat{x}_n,\, \hat{p}_n = -i\hbar\frac{\partial}{\partial x_n}$$

$$\downarrow$$

$$\hat{a}_n,\, \hat{a}_n^\dagger \text{ with } \left[\hat{a}_n,\, \hat{a}_m^\dagger\right] = \delta_{n,m}$$

$$\downarrow$$

$$\hat{a}_q = \sum_n \hat{a}_n e^{-iqn},\; \hat{a}_q^\dagger = \sum_n \hat{a}_n^\dagger e^{iqn}$$

Where we've been and where we are going

$$\hat{H} = \int_q \left[\tilde{A}(q)\hat{b}_q^\dagger \hat{b}_q + \text{H.c.}\right]$$

$$x_n,\, p_n \longrightarrow \hat{x}_n,\, \hat{p}_n = -i\hbar\frac{\partial}{\partial x_n}$$

$$\downarrow$$

$$\hat{a}_n,\, \hat{a}_n^\dagger \text{ with } \left[\hat{a}_n,\, \hat{a}_m^\dagger\right] = \delta_{n,m}$$

$$\downarrow$$

$$\hat{a}_q = \sum_n \hat{a}_n e^{-iqn},\, \hat{a}_q^\dagger = \sum_n \hat{a}_n^\dagger e^{iqn} \longrightarrow \hat{b}_q = $$ linear combination of $\hat{a}$ and $\hat{a}^\dagger$

Bogoliubov transformation

$$\begin{cases} \hat{a}_q = & u_q \hat{b}_q + v_q \hat{b}^\dagger_{-q} \\ \hat{a}^\dagger_q = & u_q \hat{b}^\dagger_q + v_q \hat{b}_{-q} \end{cases}$$

$$\left[\hat{a}_q, \hat{a}^\dagger_p\right] = \left[u_q \hat{b}_q + v_q \hat{b}^\dagger_{-q}, u_p \hat{b}^\dagger_p + v_p \hat{b}_{-p}\right]$$

$$= u_q u_p \underbrace{\left[\hat{b}_q, \hat{b}^\dagger_p\right]}_{2\pi\delta(q-p)} + u_q v_p \underbrace{\left[\hat{b}_q, \hat{b}_{-p}\right]}_{=0} + v_q u_p \underbrace{\left[\hat{b}^\dagger_{-q}, \hat{b}^\dagger_p\right]}_{=0} + v_q v_p \underbrace{\left[\hat{b}^\dagger_{-q}, \hat{b}_{-p}\right]}_{-2\pi\delta(q-p)}$$

$$= 2\pi(u_q^2 - v_q^2)\delta(q-p)$$

$$\boxed{u_q^2 - v_q^2 = 1}$$

Bogoliubov transformation

- To resolve the constraint $u_q^2 - v_q^2 = 1$ once and for all, we introduce

$$\begin{cases} u_q = \cosh \lambda_q \\ v_q = \sinh \lambda_q \end{cases} \qquad \begin{cases} \hat{a}_q = & \cosh(\lambda_q)\, \hat{b}_q + \sinh(\lambda_q)\, \hat{b}^\dagger_{-q} \\ \hat{a}^\dagger_q = & \cosh(\lambda_q)\, \hat{b}^\dagger_q + \sinh(\lambda_q)\, \hat{b}_{-q} \end{cases}$$

- The next step is to plug in into the Hamiltonian

$$\hat{H} = \int_q \left[A(q)\hat{a}^\dagger_q \hat{a}_q + B(q)\hat{a}_q\hat{a}_{-q} + \text{H.c.} \right],$$

which leads to unpleasant algebra (exercise for you).

Bogoliubov transformation

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- Result

$$\hat{H} = \int_q \left[\tilde{A}(q) \hat{b}^\dagger_q \hat{b}_q + \tilde{B}(q) \hat{b}_q \hat{b}_{-q} + \text{H.c.} \right],$$

$$\begin{cases} \tilde{A}(q) = \cosh(2\lambda_q) A(q) + \sinh(2\lambda_q) B(q) \\ \tilde{B}(q) = \cosh(2\lambda_q) B(q) + \sinh(2\lambda_q) A(q) \end{cases}$$

Bogoliubov transformation

- To resolve the constraint $u_q^2 - v_q^2 = 1$ once and for all, we introduce

$$\begin{cases} u_q = \cosh \lambda_q \\ v_q = \sinh \lambda_q \end{cases} \qquad \begin{cases} \hat{a}_q = \cosh(\lambda_q)\,\hat{b}_q + \sinh(\lambda_q)\,\hat{b}^\dagger_{-q} \\ \hat{a}^\dagger_q = \cosh(\lambda_q)\,\hat{b}^\dagger_q + \sinh(\lambda_q)\,\hat{b}_{-q} \end{cases}$$

- Result

$$\tanh(2\lambda_q) = -\frac{B(q)}{A(q)} = \frac{\frac{\hbar\omega}{2}[1-\cos(qa)] - \frac{\hbar\omega}{4}}{\frac{\hbar\omega}{2}[1-\cos(qa)] + \frac{\hbar\omega}{4}} + \mathrm{H.c.}\Big] ,$$

$$\begin{cases} \tilde{A}(q) = \hbar\omega \left|\sin\left(\frac{qa}{2}\right)\right| \text{ and } \tilde{B}(q) \equiv 0 \begin{matrix} B(q) \\ A(q) \end{matrix} \end{cases}$$

Final results

$$\hat{H} = \int_q \left[\tilde{A}(q)\hat{b}_q^\dagger \hat{b}_q + \text{H.c.}\right] \equiv \int_q \underbrace{2\tilde{A}(q)}_{\hbar\omega_q} \left(\hat{b}_q^\dagger \hat{b}_q + \frac{1}{2}\right)$$

$$\omega_q = 2\omega \left|\sin \frac{qa}{2}\right|$$

Remarkably, quantum and classical phonons have identical dispersion relations!