Recitation 5 Notes

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   c. Reciprocal Lattice Vectors

1. N-Coupled Periodic Oscillators Review

$$u(s,t) = u_0 e^{iksa-i\omega t}$$

Dispersion Relationship

$$\omega^2(k) = \frac{2K}{m}(1-\cos(ka))$$

In the long wavelength limit:

$$\omega(k) \cong \sqrt{\frac{K}{m}}ka$$

Elastic Modulus & Group Velocity
In the long wavelength or continuum limit:

$$v_g = \frac{d\omega}{dk} = \sqrt{\frac{K}{m}}a$$
$$E = \rho v_g^2$$
$$\rho \cong \frac{m}{a^3}$$
$$E \cong \frac{m}{a^3}\frac{K}{m}a^2 \cong \frac{K}{a}$$

2. Periodic Potentials Preview
   a. Conserved Quantities
      In periodic systems, the translation operator $\hat{T}_a$ commutes with the Hamiltonian $\hat{H}$. Since $\hat{H}$ and $\hat{T}_a$ are both time independent, this means that both energy and the eigenvalues of $\hat{T}_a$ are conserved quantities.
      The eigenvalues of $\hat{T}_a$ are e^{ika}, but since k, the reciprocal space wave number, is the only variable, we can alternatively consider that k is conserved. Multiplying this value by $\hbar$ we define the quantity $\hbar k$ as the crystal momentum. Note this is different from the regular momentum as the momentum operator $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ does not commute with $\hat{H}$ in periodic systems. Thus the regular momentum of an electron in a periodic potential is not conserved.
   b. Bloch Theorem
      For periodic potentials, the wave functions of particles take on the following form.

$$f_{n\vec{k}}\left(\vec{r}+\vec{R}\right) = f_{n\vec{k}}\left(\vec{r}\right)$$
$$u_{n,\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} f_{n\vec{k}}\left(\vec{r}\right)$$

or

$$u_{n,\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}u_{n,\vec{k}}(\vec{r})$$

c. Reciprocal Lattice Vectors

$$\vec{b}_1 = \frac{2\pi(\vec{a}_2 \times \vec{a}_3)}{\left(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right)} \quad \vec{b}_2 = \frac{2\pi(\vec{a}_3 \times \vec{a}_1)}{\left(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right)} \quad \vec{b}_3 = \frac{2\pi(\vec{a}_1 \times \vec{a}_2)}{\left(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right)}$$

e.g. Rectangular Lattice

Find the reciprocal lattice vectors for the following rectangular real space lattice:

$$\vec{a}_1 = a\begin{bmatrix}1\\0\\0\end{bmatrix} \vec{a}_2 = b\begin{bmatrix}0\\1\\0\end{bmatrix} \vec{a}_3 = c\begin{bmatrix}0\\0\\1\end{bmatrix}$$

$$\vec{a}_2 \times \vec{a}_3 = \det\begin{vmatrix}\hat{\imath} & \hat{\jmath} & \hat{k}\\0 & b & 0\\0 & 0 & c\end{vmatrix}$$

$$\vec{a}_2 \times \vec{a}_3 = (b\cdot c - 0\cdot 0)\hat{\imath} - (0\cdot c - 0\cdot 0)\hat{\jmath} + (0\cdot 0 - 0\cdot b)\hat{k}$$

$$\vec{a}_2 \times \vec{a}_3 = bc\begin{bmatrix}1\\0\\0\end{bmatrix}$$

$$\vec{a}_3 \times \vec{a}_1 = \det\begin{vmatrix}\hat{\imath} & \hat{\jmath} & \hat{k}\\0 & 0 & c\\a & 0 & 0\end{vmatrix}$$

$$\vec{a}_3 \times \vec{a}_1 = (0\cdot 0 - 0\cdot c)\hat{\imath} - (0\cdot 0 - a\cdot c)\hat{\jmath} + (0\cdot 0 - a\cdot 0)\hat{k}$$

$$\vec{a}_3 \times \vec{a}_1 = ac\begin{bmatrix}0\\1\\0\end{bmatrix}$$

$$\vec{a}_1 \times \vec{a}_2 = \det\begin{vmatrix}\hat{\imath} & \hat{\jmath} & \hat{k}\\a & 0 & 0\\0 & b & 0\end{vmatrix}$$

$$\vec{a}_1 \times \vec{a}_2 = (0\cdot 0 - b\cdot 0)\hat{\imath} - (a\cdot 0 - 0\cdot 0)\hat{\jmath} + (a\cdot b - 0\cdot 0)\hat{k}$$

$$\vec{a}_1 \times \vec{a}_2 = ab\begin{bmatrix}0\\0\\1\end{bmatrix}$$

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = (a\cdot bc) + (0\cdot 0) + (0\cdot 0) = abc$$

$$\vec{b}_1 = \frac{2\pi(\vec{a}_2 \times \vec{a}_3)}{\left(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right)} = \frac{2\pi bc}{abc}\begin{bmatrix}1\\0\\0\end{bmatrix} = \frac{2\pi}{a}\begin{bmatrix}1\\0\\0\end{bmatrix}$$

$$\vec{b}_2 = \frac{2\pi(\vec{a}_3 \times \vec{a}_1)}{\left(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right)} = \frac{2\pi ac}{abc}\begin{bmatrix}0\\1\\0\end{bmatrix} = \frac{2\pi}{b}\begin{bmatrix}0\\1\\0\end{bmatrix}$$

$$\vec{b}_3 = \frac{2\pi(\vec{a}_1 \times \vec{a}_2)}{\left(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right)} = \frac{2\pi ab}{abc}\begin{bmatrix}0\\0\\1\end{bmatrix} = \frac{2\pi}{c}\begin{bmatrix}0\\0\\1\end{bmatrix}$$