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# Band Theory

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*Consider an electron in a 1-dimensional system with periodic potential $V(x)$. Argue that the potential can be written as:*

$$V(x) = \sum_K V_K \exp(iKx). \tag{1}$$

*Which values of $K$ are summed over?*

$V(x)$ is a periodic function and hence can be represented as a Fourier series. The terms required are those with the periodicity of the lattice: i.e., $K$ vectors in the reciprocal lattice.

*We will consider the effect of one component of the periodic potential. Assuming $V(x)$ is real and symmetric, show that $V_K = V_{-K} = V_K^*$.*

$$\int_{-\pi/a}^{\pi/a} V(x)\exp(-iK'x)\mathrm{d}x = \sum_K \int_{-\pi/a}^{\pi/a} \mathrm{d}x V_K \exp(iKx)\exp(-iK'x) = \frac{2\pi}{a}\sum_K V_K \delta_{K,K'} \tag{2}$$

$$\implies V_K = \frac{a}{2\pi}\int V(x)\exp(-iKx)\mathrm{d}x, \tag{3}$$

where $a$ is the lattice constant. Making the substitution $y = -x$, and remembering that we get a minus sign from switching the limits,

$$\implies V_K = \frac{a}{2\pi}\int V(-y)\exp(iKy)\mathrm{d}y. \tag{4}$$

Now use $V(-y) = V(y)$, and change the dummy variable $y$ back to $x$.

$$\implies V_K = \frac{a}{2\pi}\int V(x)\exp(iKx)\mathrm{d}x, \tag{5}$$

$$\implies V_K = V_{-K}. \tag{6}$$

By taking the conjugate of Eq. 3, we immediately obtain $V_{-K} = V_K^*$.

*Thus our perturbation becomes $V(x) = V_K(\exp(iKx)+\exp(-iKx))$. We can write the Schrödinger equation in matrix from as*

$$\langle\Psi|H_0|\Psi\rangle + \langle\Psi|V(x)|\Psi\rangle = E \tag{7}$$

*Our unperturbed eigenstates are plane waves, $|\Psi_k(x)\rangle$. Argue that*

$$\langle\Psi_k|V(x)|\Psi_k'\rangle = V_K\sum_K V_K\delta(k-k'-K). \tag{8}$$

$$\langle\Psi_k|V(x)|\Psi_k'\rangle = \int \mathrm{d}x \frac{\exp(-ikx)}{(2\pi)^{1/2}}V(x)\frac{\exp(ik'x)}{(2\pi)^{1/2}} = \frac{1}{2\pi}\sum_K V_K\int \mathrm{d}x\exp(-i(k-k'-K)x) \tag{9}$$

$$\implies \langle\Psi_k|V(x)|\Psi_k'\rangle = \sum_K V_K\delta(k-k'-K). \tag{10}$$

*The Hamiltonian only acts to connect states with $k - k' = \pm K$. Unfortunately, this is still an infinite number of states. Ideally, we would like to restrict ourselves to pairs of states with $|k| \approx |k'| \approx |K|/2$, as this makes the problem easy to solve. Why might this be a reasonable assumption? Think about the second order term in perturbation theory: is it large if the unperturbed states have very different energies?*

Perturbation theory tends to couple states of similar energies: in particular the first order perturbation to the wavefunction and the second order perturbation to the energy vary as $1/\Delta E$.

*Hence show that a state given by $|\Psi(x)\rangle = a|\Psi_k(x)\rangle + b|\Psi_{k-K}(x)\rangle$ obeys the Schrödinger equation:*

$$\begin{pmatrix} \frac{\hbar^2 k^2}{2m} & V_K \\ V_K & \frac{\hbar^2 (k-K)^2}{2m} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = E \begin{pmatrix} a \\ b \end{pmatrix} \tag{11}$$

$H_0$ simply gives the unperturbed energies of the plane waves, and doesn't connect different plane wave states.

$$\langle \Psi_k(x)|H_0|\Psi_k(x)\rangle = \frac{\hbar^2 k^2}{2m}, \tag{12}$$

$$\langle \Psi_{k-K}(x)|H_0|\Psi_{k-K}(x)\rangle = \frac{\hbar^2 (k-K)^2}{2m}, \tag{13}$$

$$\langle \Psi_k(x)|H_0|\Psi_{k-K}(x)\rangle = 0. \tag{14}$$

We can simply use the relations derived in Eq. 10 to get the matrix elements for the perturbation between the states involved. Ignoring any irrelevant constant term in the energy, we obtain:

$$\langle \Psi_k(x)|V(x)|\Psi_k(x)\rangle = 0, \tag{15}$$

$$\langle \Psi_{k-K}(x)|V(x)|\Psi_{k-K}(x)\rangle = 0, \tag{16}$$

$$\langle \Psi_k(x)|V(x)|\Psi_{k-K}(x)\rangle = \langle \Psi_{k-K}(x)|V(x)|\Psi_k(x)\rangle = V_K. \tag{17}$$

Combining these with Eq. 7 we obtain the desired matrix equation.

*Solve for the eigenvalues, expanding to quadratic order in $\delta = k - K/2$. What are the eigenvectors if $k$ lies on the Brillouin zone boundary at $K/2$? What sort of waves are these?*

Eigenvalues are given by:

$$\left(\frac{\hbar^2 k^2}{2m} - E\right)\left(\frac{\hbar^2 (k-K)^2}{2m} - E\right) - V_k^2 = 0. \tag{18}$$

$$\implies E = \frac{1}{2}\frac{\hbar^2}{2m}\left(k^2 + (k-K)^2 \pm \left(\left(k^2 + (k-K)^2\right)^2 + 4V_K^2\left(\frac{2m}{\hbar^2}\right)^2\right)^{0.5}\right) \tag{19}$$

Let $\delta = k - K/2$:

$$\implies E = \frac{\hbar^2}{4m}\left((\delta + K/2)^2 + (\delta - K)^2 \pm \left(4\delta^2 k^2 + V_K^2\left(\frac{2m}{\hbar^2}\right)^2\right)^{0.5}\right). \tag{20}$$

Expanding to lowest order in $\delta$:

$$\implies E = \frac{\hbar^2}{2m}\left(\delta^2 + (K/2)^2\right) \pm V_K\left(1 + \frac{\hbar^4 K^2 \delta^2}{8m^2 V_K^2}\right). \tag{21}$$

We note that this is quadratic in $\delta$.
For $\delta = 0$, $E = \frac{\hbar^2 k^2}{2m} \pm V_k$, which gives $|\Psi(x)\rangle = \frac{1}{\sqrt{2}}\left(|\Psi_k(x)\rangle \pm |\Psi_{-k}(x)\rangle\right)$. These are standing waves.