One Dimensional Lattice: Weak-Coupling Limit

In Lectures 37 and 38 we considered the strong coupling limit, like tunneling in H_2^+. Now we will look at the periodic lattice as a perturbation on the free particle.

See Baym "Lectures on Quantum Mechanics" pages 237-241.

Each atom in a lattice is represented by a 1-D V(x) that could bind an unspecified number of electronic states:

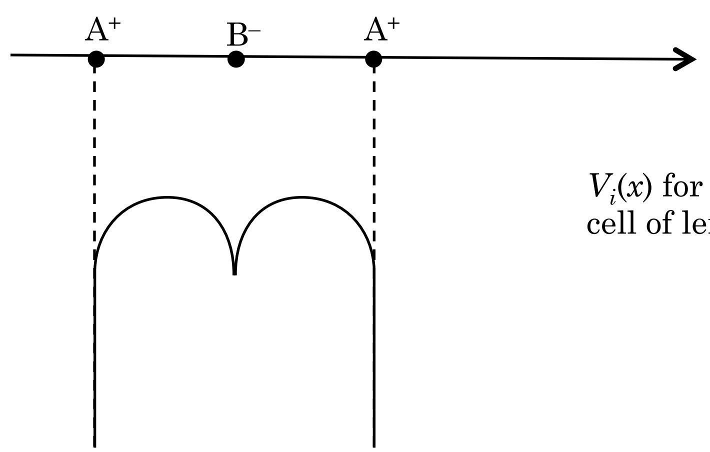
Now consider a lattice that could consist of two or more different types of atoms.

Periodic structure: repeated for each "unit cell", of length ℓ.

Consider a finite lattice (N atoms), but impose a periodic (head-to-tail) boundary condition.

$L = N\ell$

For each unit cell:



$V_i(x)$ for i-th unit cell of length ℓ

This is an infinitely repeated finite interval: Fourier Series

$$V(x) = \sum_{n=-\infty}^{\infty} e^{iKnx} V_n$$

$$K = \frac{2\pi}{\ell} \quad \text{"reciprocal lattice vector"}$$

V_n is the (possibly complex) Fourier coefficient of the part of $V(x)$ that *looks like* a free particle state with wave-vector Kn (momentum $\hbar Kn$). Note that Kn is larger than the largest k (shortest λ) free-particle state that can be supported by a lattice of spacing ℓ.

$$Kn = n\frac{2\pi}{\ell} \quad , \qquad \text{first Brillouin Zone for } k\text{:}$$

$$-\frac{\pi}{\ell} \le k \le \frac{\pi}{\ell}$$

We will see that the lattice is able to exchange momentum in quanta of $\hbar nK$ with the free particle. In 3-D, $\vec{K}$ is a vector.

To solve for the effect of $V(x)$ on a free-particle, we use perturbation theory. The free particle basis states are weakly perturbed by the periodic lattice.

1. Define the basis set.

$$\left.\begin{aligned}
\mathbf{H}^{(0)} &= \frac{\mathbf{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V^{(0)} \\
V^{(0)} &= \text{constant} \\
\psi_k^{(0)} &= L^{-1/2}e^{ikx}
\end{aligned}\right\} \text{free particle}$$

$$\left[\text{Normalization: } \int_0^L dx\left|\psi_k^{(0)}\right|^2 = L(1/L) = 1\right]$$

one particle per L

$$E_k^{(0)} = \frac{\hbar^2 k^2}{2m} + V^{(0)} \longleftarrow \text{ignore}$$

2. $$\mathbf{H}^{(1)} = \sum_{n=-\infty}^{\infty} e^{iKn}V_n$$

$$\text{Matrix elements: } H_{k'k}^{(1)} = \int_0^L dx\Big[\overbrace{L^{-1/2}e^{-ik'x}}^{\psi_{k'}^{(0)*}}\Big]\left[\sum_n e^{iKnx}V_n\right]\left[L^{-1/2}e^{ikx}\right]$$

$$H_{k'k}^{(1)} = \frac{1}{L}\int_0^L dx\sum_n e^{ix(k+Kn-k')}V_n$$

$$\boxed{\begin{aligned}&\text{integral} = 0 \text{ if } k + Kn - k' \ne 0\\ &\qquad \therefore k' = k + Kn \quad \text{selection rule}\end{aligned}}$$

$$H_{k'k}^{(1)} = \frac{1}{L}L\sum_n V_n\delta_{k',k+Kn} = \sum_n V_n\delta_{k',k+Kn}$$

Must be careful about $H^{(1)}_{kk'}$ $\left(\text{relative to } H^{(1)}_{k'k}\right)$. Return to definition.

$$H^{(1)}_{kk'} = \frac{1}{L}\int_0^L dx \sum_n e^{ix(-k+Kn+k')} V_n = \sum_n V_n \delta_{k',k-Kn}$$

but Hermitian $\mathbf{H}$ requires $H^{(1)}_{kk'} = H^{(1)*}_{k'k}$

$$\therefore \sum_n V_n \delta_{k',k-Kn} = \sum_n V_n^* \delta_{k',k+Kn}$$

true if $V_n = V^*_{-n}$.

So now that we have the matrix elements of $\mathbf{H}^{(0)}$ and $\mathbf{H}^{(1)}$, the problem is essentially solved. All that remains is to plug into perturbation theory and arrange the results.

3. Solve for $\psi_k = \psi_k^{(0)} + \psi_k^{(1)}$

$$\psi_k^{(0)} = L^{-1/2} e^{ikx}$$

$$\psi_k^{(1)} = L^{-1/2} \sum_n{}' \frac{H^{(1)}_{kk'} \overbrace{e^{ik'x}}^{\psi^{(0)}_{k'}}}{E_k^{(0)} - E_{k'}^{(0)}} = L^{-1/2} \sum_n{}' \frac{\overbrace{V_n \delta_{k',k-Kn}}^{H^{(1)}_{k,k'}} e^{ik'x}}{E_k^{(0)} - E^{(0)}_{\underbrace{\boxed{k-Kn}}_{k' = k-Kn}}} \quad (\Sigma' \text{ means } k' \neq k)$$

$$\psi_k^{(1)} = L^{-1/2} \sum_n{}' \frac{V_n e^{i(k-Kn)x}}{E_k^{(0)} - E_{k-Kn}^{(0)}}$$

imposing Kronecker δ-fn restriction on $e^{ik'x}$

Now be careful to express $\psi_k^{(1)*}$ correctly.

$$\psi_k^{(1)*} = L^{-1/2} \sum_n{}' \frac{V_n^* e^{-i(k-Kn)x}}{E_k^{(0)} - E_{k-Kn}^{(0)}}$$

$$V_n^* = V_{-n}$$

$$\psi_k^{(1)*} = L^{-1/2} \sum_n{}' \frac{V_{-n} e^{-i(k-Kn)x}}{E_k^{(0)} - E_{k-Kn}^{(0)}} = L^{-1/2} \sum_{-n}{}' \frac{V_n e^{-i(k+Kn)x}}{E_k^{(0)} - E_{k+Kn}^{(0)}}$$

replace n by –n

But n is just a dummy index and sum is –∞ to ∞, so we can replace $-n$ by n.

4. Use ψ_k and ψ_k^* to compute $E_k = E_k^{(0)} + E_k^{(1)} + E_k^{(2)}$.

Rather than use the usual formula for $E^{(2)}$, go back to the λ^n formulation of perturbation theory.

$$E_k = \lambda^0 E_k^{(0)} + \lambda^1 E_k^{(1)} + \lambda^2 E_k^{(2)} = \left\langle \psi_k \middle| \lambda^0 \mathbf{H}^{(0)} + \lambda^1 \mathbf{H}^{(1)} \middle| \psi_k \right\rangle$$

Retain terms only through λ^2

$$E_k = \frac{1}{L}\int_0^L dx \Bigg[\underbrace{e^{-ikx}}_{\psi_k^{(0)*}} + \lambda \overbrace{\sum_n{}' \frac{V_n e^{-i(k+Kn)x}}{E_k^{(0)} - E_{k+Kn}^{(0)}}}^{\psi_k^{(1)*}} \Bigg] \Bigg[-\underbrace{\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\mathbf{H}^{(0)}} + \lambda \underbrace{\sum_m V_m e^{iKmx}}_{\mathbf{H}^{(1)}} \Bigg]$$
$$\times \Bigg[\underbrace{e^{ikx}}_{\psi_k^{(0)}} + \lambda \underbrace{\sum_{n'}{}' \frac{V_{n'} e^{i(k-Kn')x}}{E_k^{(0)} - E_{k-Kn'}^{(0)}}}_{\psi_k^{(1)}} \Bigg]$$

$$E_k^{(0)} = \lambda^0 \frac{1}{L}\left[-\frac{\hbar^2}{2m}\left(-k^2\right)L \right] = \lambda^0 \frac{\hbar^2 k^2}{2m} \qquad \left[\text{recall } \frac{d^2}{dx^2} e^{ikx} = -k^2 e^{ikx} \right]$$

$$E_k^{(1)} = \lambda^1 \frac{1}{L}\left[\int dx\, e^{-ikx} \sum_m e^{iKmx} V_m e^{ikx} + 2 \text{ terms involving } \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \right) \right],$$

and also retain one of the $\sum'$ sums (that excludes $n=0$)

We will get to the λ^2 equation on the next page.
For $E_k^{(1)}$: for 1st term, only the $m = 0$ term in the sum gives a nonzero integral. For 2nd terms, need an n or $n' = 0$ term from the sum, but these are excluded by the $\sum'$ sums.

$$E_k^{(1)} = \lambda^1 \frac{1}{L} L V_0 = \lambda^1 V_0$$

This is basically telling us the location of the bottom of the band relative to "vacuum".

Three ways to get λ^2 terms, two ways involve the $\mathbf{H}^{(1)}$ term, and one involves the $\mathbf{H}^{(0)}$ term. The $\mathbf{H}^{(0)}$ term requires $n = -n'$ ..

$$E_k^{(2)} = \frac{1}{L}\lambda^2 \left[\int dx\, e^{-ikx} \sum_{m=-\infty}^{\infty} V_m e^{iKmx} \sum_{n'=-\infty}^{\infty}{}' \frac{V_{n'} e^{i(k-Kn')x}}{E_k^{(0)} - E_{k-Kn'}^{(0)}} + \int dx \sum_{n\neq 0}{}' \frac{V_n e^{-i(k+Kn)x}}{E_k^{(0)} - E_{k+Kn}^{(0)}} \left(\sum_m V_m e^{iKm} \right) e^{ikx} \right]$$

needed to make integral non-zero

1st term $\quad 0 = -k + Km + k - Kn'$, requires m = n′

2nd term $\quad 0 = -k - Kn + Km + k$, requires m = n

$$E_k^{(2)} = \frac{1}{L}\lambda^2 \left[\int dx \sum_m{}' \frac{V_m^2}{E_k^{(0)} - E_{k-Km}^{(0)}} + \int dx \sum_m{}' \frac{V_m^2}{E_k^{(0)} - E_{k+Km}^{(0)}} \right]$$

These are both the same sum, the $\int dx$ integral gives L. Now we simplify this.

$$E_k^{(2)} = 2\lambda^2 \sum_{n=-\infty}^{\infty}{}' \frac{V_n^2}{E_k^{(0)} - E_{k+Kn}^{(0)}}$$

Combine terms for n and $-n$ and sum $\sum_{n=1}^{\infty}$

Solve for the energy denominator terms

$$E_k^{(0)} - E_{k\pm Kn}^{(0)} = \frac{\hbar^2}{2m}\left[k^2 - (k \pm Kn)^2\right] = -\frac{\hbar^2 Kn}{2m}\left[Kn \pm 2k\right]$$

Combine the energy denominators

$$\frac{1}{E_k^{(0)} - E_{k+Kn}^{(0)}} + \frac{1}{E_k^{(0)} - E_{k-Kn}^{(0)}} = \frac{4m}{\hbar^2}\frac{1}{K^2n^2 - 4k^2}$$

Assemble $E_k^{(2)}$

$$E_k^{(2)} = \frac{-8m}{\hbar^2}\sum_{n=1}^{\infty}\frac{V_n^2}{K^2n^2 - 4k^2}.$$

But there are many zeroes in this denominator as n goes from $1 \to \infty$.

Must use degenerate perturbation theory for *each* small denominator.

Recall, for the 2-level problem

$$\begin{pmatrix} E_k & V \\ V & E_{k'} \end{pmatrix} \longrightarrow E_{\pm} = \frac{E_k + E_{k'}}{2} \pm \left[\left(\frac{E_k - E_{k'}}{2}\right)^2 + V^2\right]^{1/2}$$

$$E_k = \frac{\hbar^2 k^2}{2m} + V_0 - \frac{8m}{\hbar^2}\sum_{n=1}^{\infty} \frac{V_n^2}{K^2 n^2 - 4k^2}$$

Must be negative near $k = 0$ because the lowest states are always pushed to lower energy.

zeroes at $k = \pm\frac{Kn}{2} = \pm\frac{2\pi}{2\ell}n = \pm\frac{n\pi}{\ell}$, except $n = 0$.

At $k = 0$, there are no nearby zeroes

$$\left.\frac{dE_k}{dk}\right|_{k=0} = \frac{\hbar^2 k}{m} \qquad \text{(minimum at } k = 0\text{)}$$

$$\left.\frac{d^2 E_k}{dk^2}\right|_{k=0} = \frac{\hbar^2}{m} \qquad \text{(positive curvature)}$$

just like free particle!

At $k = \pm\frac{K}{2}$, there are zeroes in the denominator, so there are gaps in the energy:

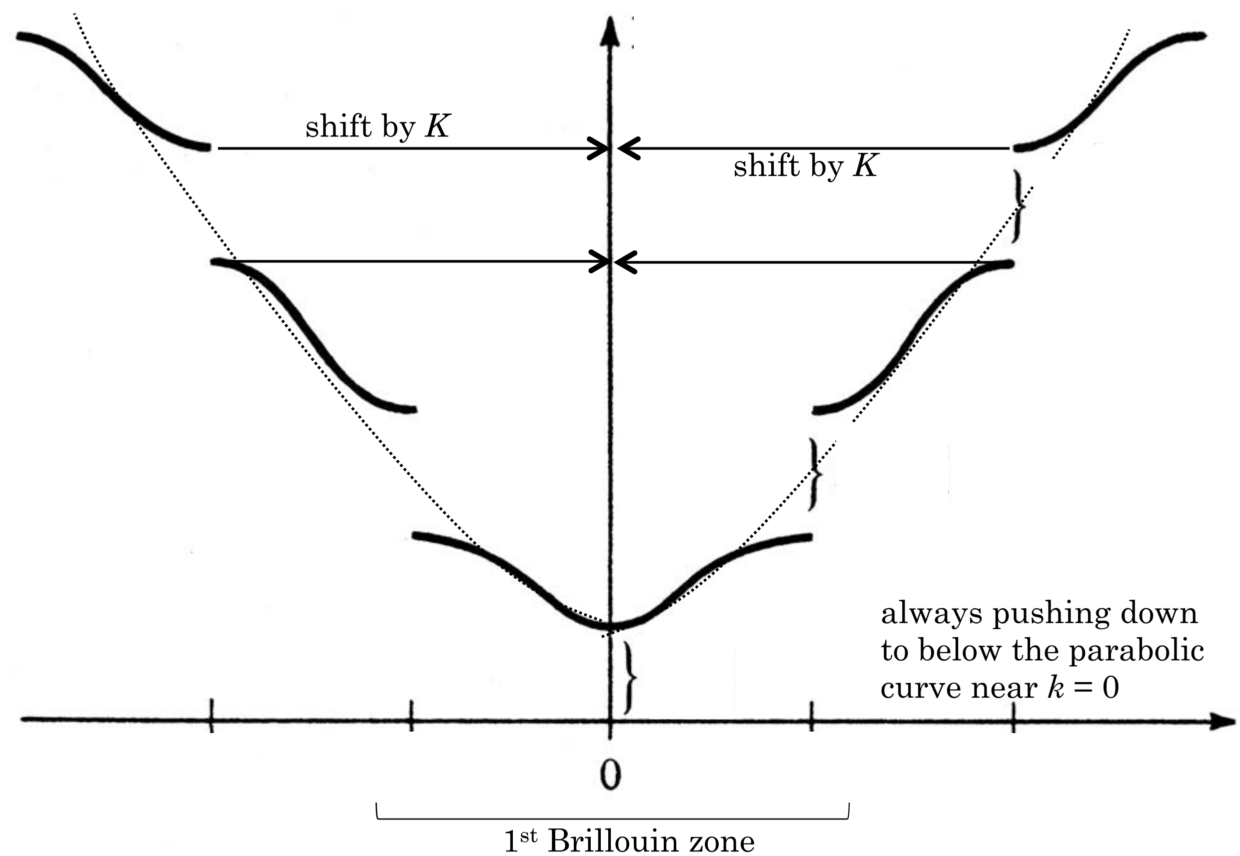
$2|\mathrm{V}_1|$ at $k = \pm\frac{K}{2}$

$2|\mathrm{V}_2|$ at $k = \pm K$

$\vdots$

$2|\mathrm{V}_n|$ at $k = \pm\frac{nK}{2}$

What does this look like?



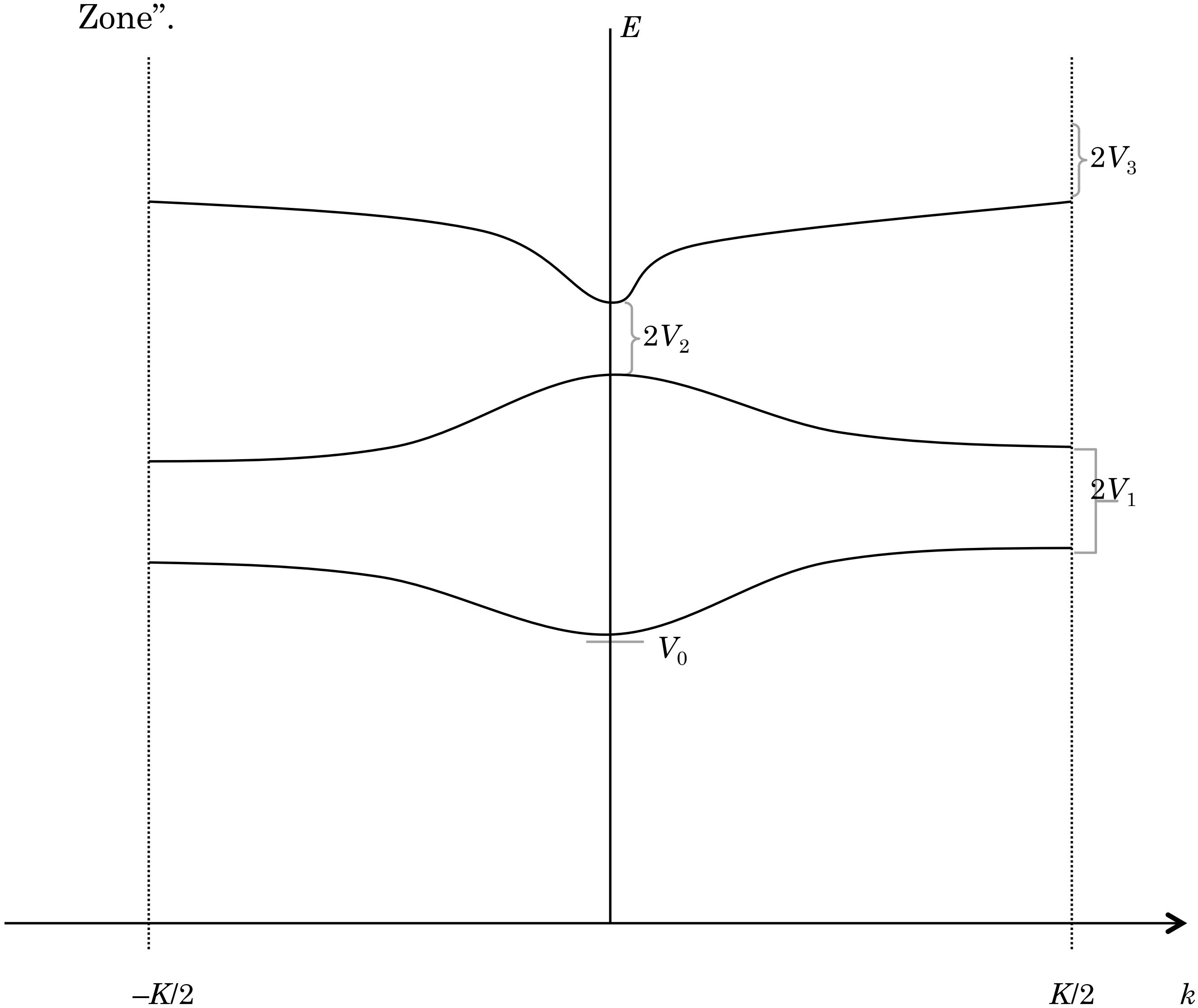
$$E = V_0 + \left(\frac{\hbar^2}{2m}\right)k^2$$

look at text Baym "Lectures on Quantum Mechanics," Benjamin (1981), page 240.

$k = \frac{\pi}{\ell}$ for the lowest energy segment of the $E_k(k)$ curve.

We know that all ψ's have been generated within $-\frac{\pi}{2\ell} \leq k \leq \frac{\pi}{2\ell}$, but there are some different values of E for the same k at each discontinuity.

But we want to shift each of the segments by an integer times K to the left or right so that each shift within the $-\frac{K}{2} \leq k \leq \frac{K}{2}$ "First Brilouin Zone".



E vs. k diagram. Curvature gives m_{eff}.

3-D diagram — gives much more information. Tells us where to find transitions allowed as a function of 3-D $\vec{k}$ vector in "reciprocal lattice" of lattice vector $\vec{K}$.

Scattering of free particle off lattice. Conservation of momentum in the sense $\vec{k}_{\text{final}} - \vec{k}_{\text{initial}} = \vec{K}$.