One Dimensional Lattice: Weak Coupling Limit

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

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

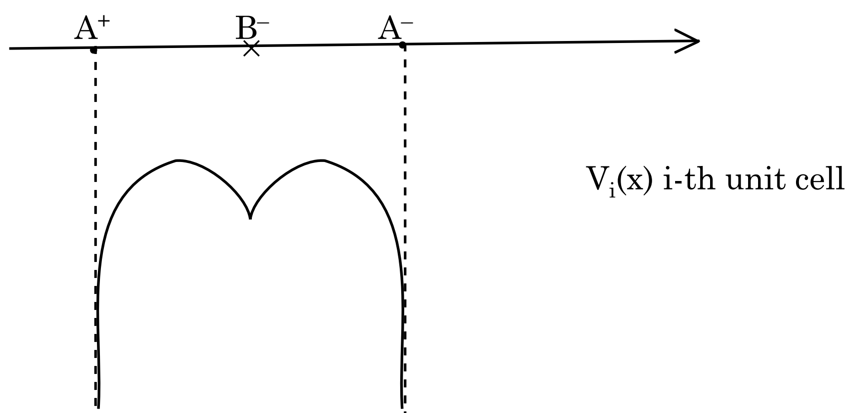
Lattice could consist of two or more different types of atoms.

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

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

$L = N\ell$

Each unit cell, eq:



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.

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

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

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.

1. Define basis set.

$$\mathbf{H}^{(0)} = \frac{\mathbf{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$V^{(0)} = \text{constant}$$

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

$$E_k^{(0)} = \frac{\hbar^2 k^2}{2m}$$

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

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

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

$$\text{integral} = 0 \text{ if } k + Kn - k' \neq 0$$
$$\therefore k' = k + Kn$$

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

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

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

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

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

$$\text{true if } V_n = V_{-n}^*$$

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 $\psi_k = \psi_k^{(0)} + \psi_k^{(1)}$

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

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

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

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

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

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

But n is just a dummy index, so 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

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

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

$$E_k^{(0)} = \lambda^1 \frac{1}{L}\left[\int dx\, e^{-ikx} \sum_m e^{iKmx} V_m e^{ikx} + 2 \text{ terms involving} \left(-\frac{\mathbf{h}^2}{2m}\frac{d^2}{dx^2} \right) \right]$$

1st term, only m = 0 term in sum gives nonzero integral.
2nd terms, need n or n′ = 0 term from sum, but these are excluded by Σ′.

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

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

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

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

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

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

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

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

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

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

But there are many zeroes in this denominator as n goes $0 \to \infty$.

Must use degenerate perturbation theory for each small denominator.

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

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

zeroes at $k = \pm\frac{Kn}{2} = \pm\frac{2\pi}{2\mathbf{l}}n = \pm\frac{n\pi}{\mathbf{l}}$ except $n = 0$

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

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

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

just like free particle!

At $k = \pm\frac{K}{2}$, there are zeroes in denominator, so there is a gap in energy of

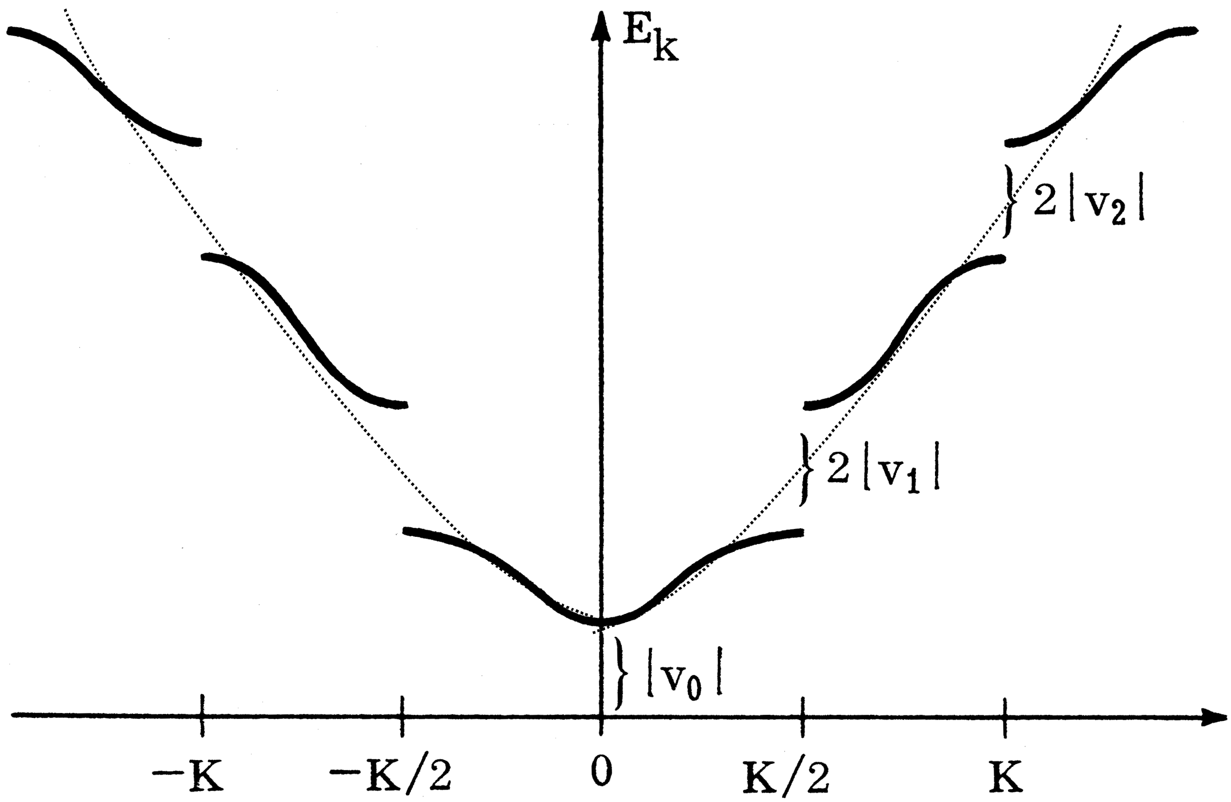
$2|V_1|$ at $k = \pm\frac{K}{2}$

$2|V_2|$ at $k = \pm K$

$\vdots$

$2|V_n|$ at $k = \pm\frac{nK}{2}$

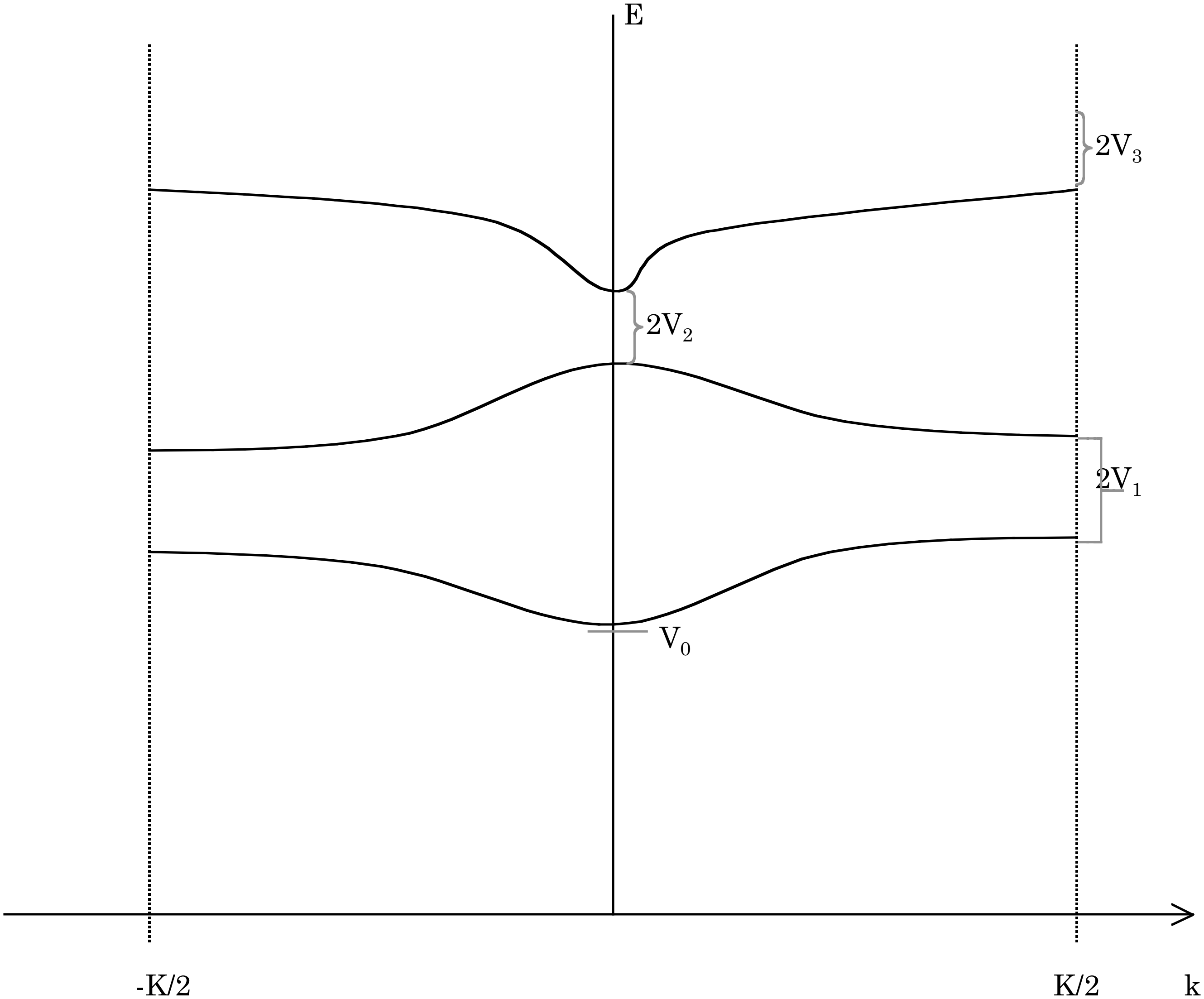
What does this look like?



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

look at text Baym page 240.

But we want to shift each of the segments by integer times K to left or right so that they all fit within the $\frac{-K}{2} \leq k \leq \frac{K}{2}$ "first Brillouin Zone".



k diagram. Curvature gives m_{eff}

3 – D k - diagram — much more information. Tells where to find allowed transitions as 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 $\vec{k}_{final} - \vec{k}_{initial} = \vec{K}$.