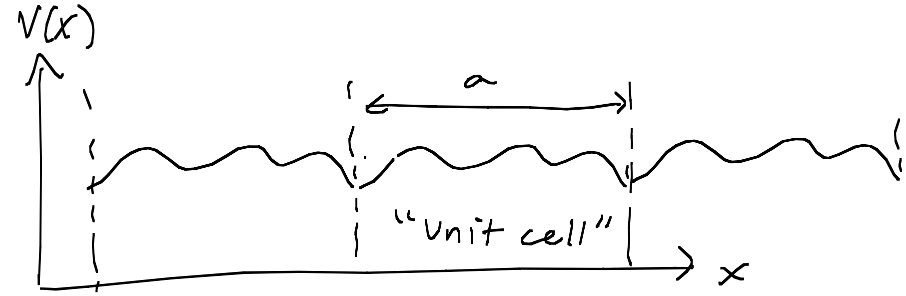
periodic potentials (a simple model for crystalline solid)



$V(x) = V(x+a)$ $\quad$ a is "lattice constant"

$= \sum_g c(g) e^{igx}$ $\quad$ $g = 0, \pm\frac{2\pi}{a}, \pm\frac{4\pi}{a}, \ldots$

(Fourier Series) $\quad$ is "reciprocal lattice number"

Our solution has the same symmetry as the potential:

$\psi(x) = e^{ikx} u(x)$ $\quad$ "Bloch wave" where $u(x) = \sum_g b(g) e^{igx}$

Schrödinger Eq:

$$-\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi$$

substitute:

$$-\frac{\hbar^2}{2m}\left(e^{ikx}u(x)\right)'' + Ve^{ikx}u(x) = Ee^{ikx}u(x)$$

Now, since $(f_1 f_2)'' = (f_1' f_2 + f_1 f_2')' = f_1'' f_2 + 2f_1' f_2' + f_1 f_2''$,

$$-\frac{\hbar^2}{2m}\left[-k^2 \cancel{e^{ikx}} u(x) + 2ik\cancel{e^{ikx}} u'(x) + \cancel{e^{ikx}} u''(x)\right] + V\cancel{e^{ikx}} u(x) = E\cancel{e^{ikx}} u(x)$$

$$-\frac{\hbar^2}{2m}\left(u'' + 2iku' - k^2 u\right) + Vu = Eu$$

$$-\frac{\hbar^2}{2m}\left(\frac{d}{dx} + ik\right)^2 u + Vu = Eu$$

because: $\quad u(x) = \sum_g b(g) e^{igx} \qquad V(x) = \sum_g c(g) e^{igx} \quad$ so $\frac{d}{dx} \to ig$:

$$-\frac{\hbar^2}{2m}\sum_g (ik+ig)^2 b(g) e^{igx} + \sum_{g'} c(g') e^{ig'x} \sum_g b(g) e^{igx} = E \sum_g b(g) e^{igx}$$

(g' has same discrete values as g but is summed over separately)

$$\frac{\hbar^2}{2m}\sum_g (k+g)^2 b(g) e^{igx} + \sum_{g'} c(g') e^{ig'x} \sum_g b(g) e^{igx} = E \sum_g b(g) e^{igx}$$

This is <u>hard</u> to solve for $b(g)$ exactly if the sums are infinite so we have to terminate them to calculate.

But first, look at the simplest case ...

When $V(x) \to 0$ (all $c(g)$'s $= 0$)

Then we retain only the periodicity of the potential:

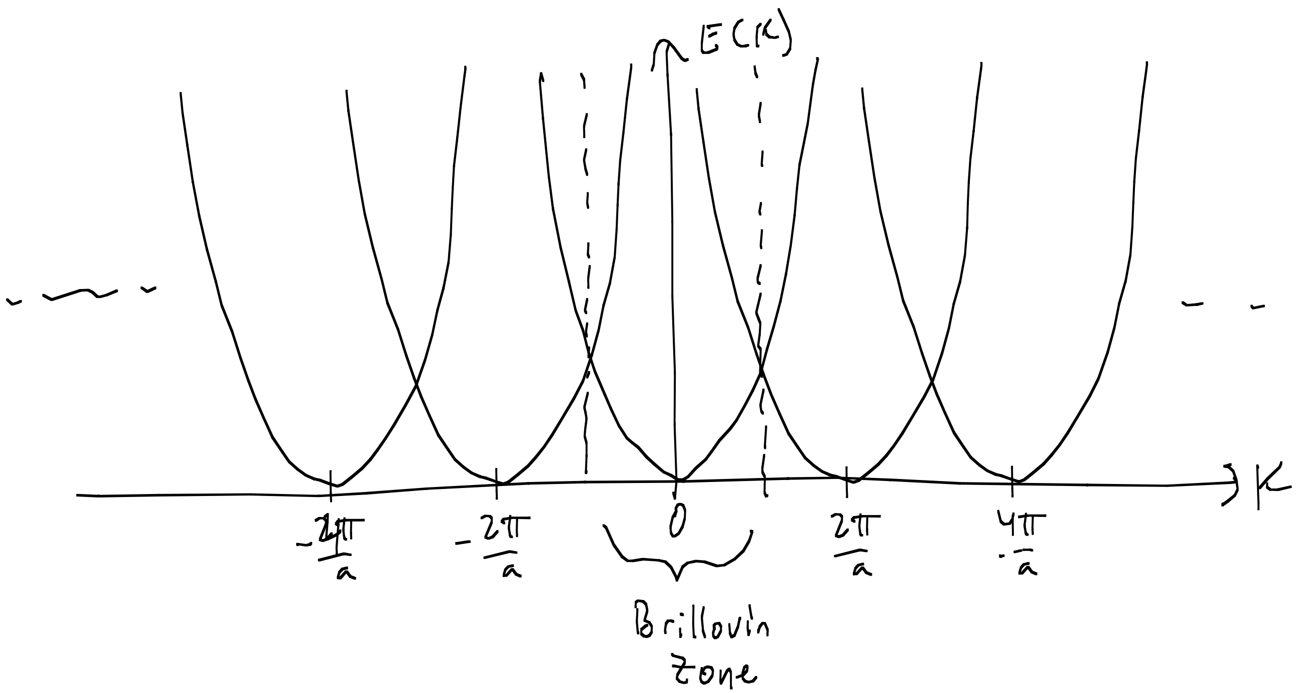
$$\frac{\hbar^2}{2m}\sum_g (k+g)^2 b(g) e^{igx} = E \sum_g b(g) e^{igx}$$

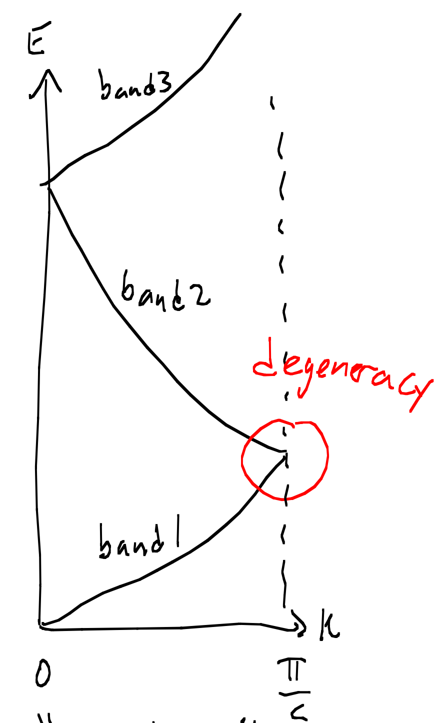
reminder:
k is continuous /
g is discrete
$(= 0, \pm\frac{2\pi}{a}, \pm\frac{4\pi}{a}, \ldots)$

because of orthonormality of basis fns,

$$E = \frac{\hbar^2}{2m}(k+g)^2 :$$

"Band structure"





Like the free-particle dispersion only repeated periodically!

"Irreducible" BZ

When $V(x) \neq 0$

Consider the degeneracy (circled in previous slide) at $k = \frac{\pi}{a}$.

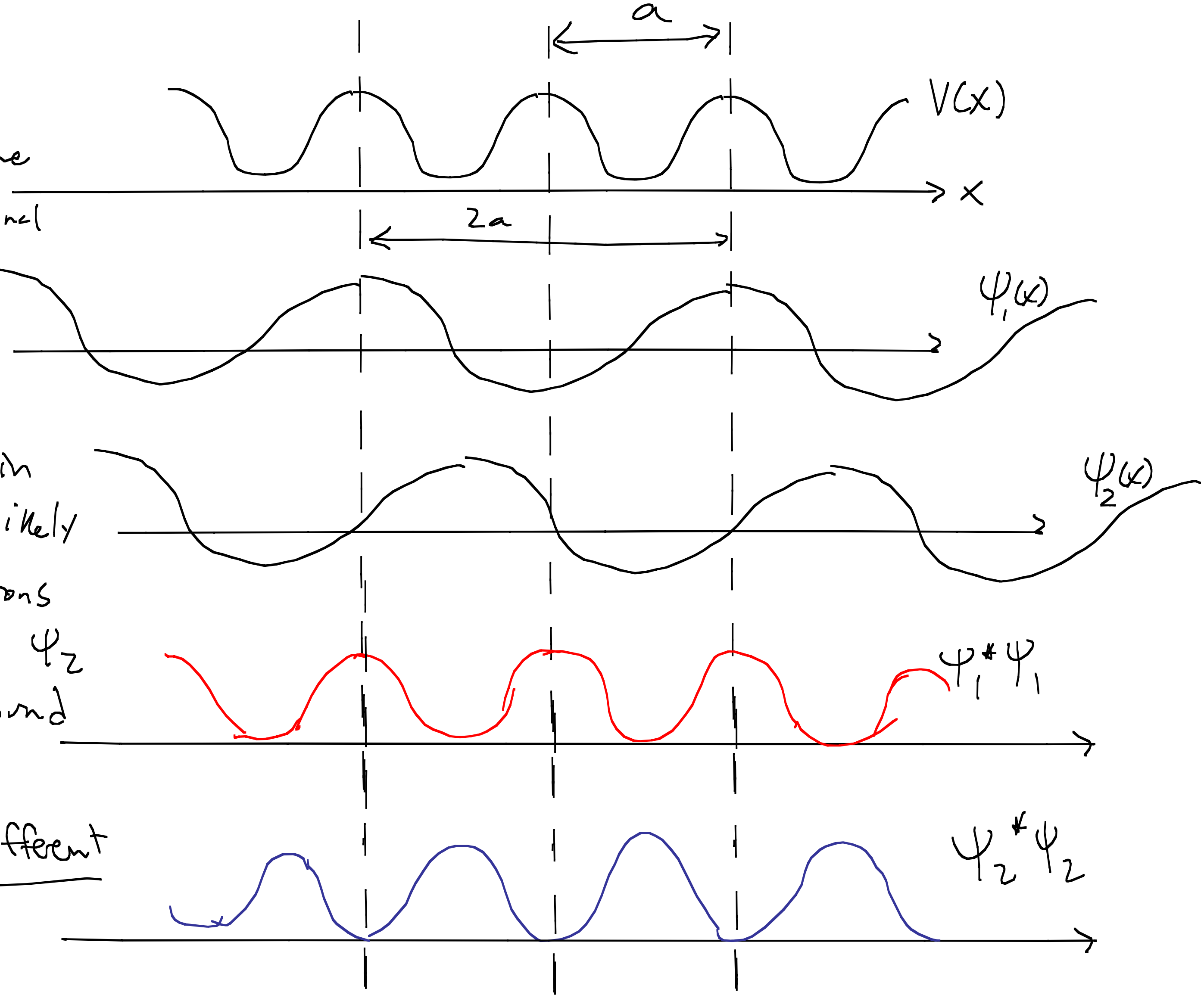
Then $\lambda = \frac{2\pi}{k} = 2a$:

ψ_1 and ψ_2 have the same wavelength, but are orthogonal as required for eigenstates.

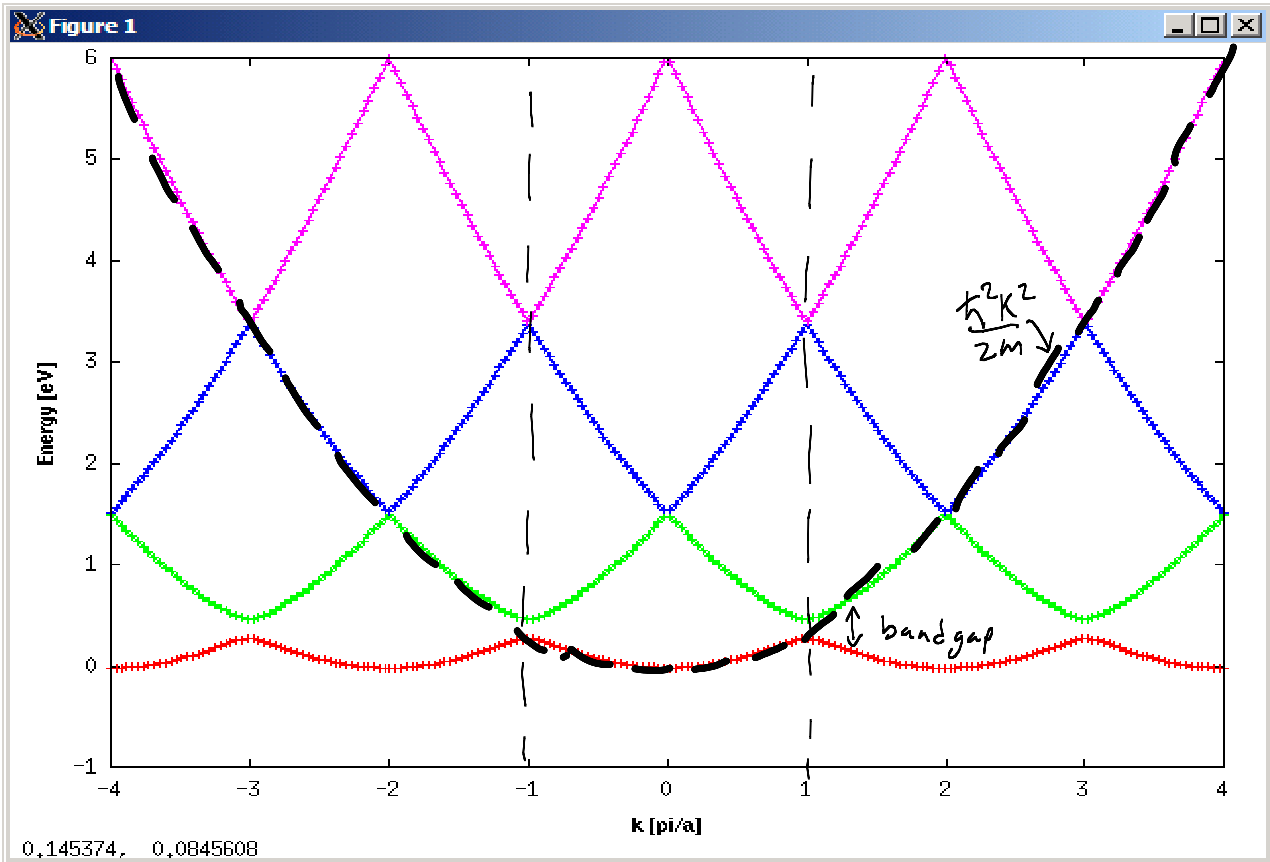
Probability density $\psi^*\psi$ shows that an electron in eigenstate ψ_1 is more likely to be found at regions where $V(x)$ is large, and ψ_2 is more likely to be found where $V(x)$ is small.

So the energies are different

i.e. degeneracy is broken!



Example: $V(x) = 0.2 \cos\frac{2\pi x}{a}$ (eV), $a = 1\,nm$



Like free electron dispersion w/ small "bandgaps" where degeneracy is lifted at Brillouin zone edge. Then, the dispersion relation is altered and so too are the dynamics!

Electrons in bands: Dynamics

Consider acceleration due to a force:

$$a = \frac{dV_g}{dt} = \frac{d}{dt}\frac{d\omega}{dK} = \frac{1}{\hbar}\frac{d}{dt}\frac{dE}{dK} = \frac{1}{\hbar}\frac{d\frac{dE}{dK}}{dK}\frac{dK}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dK^2}\frac{dp}{dt}$$

$(E = \hbar\omega)$ $\qquad$ $(p = \hbar K)$

$$= \left(\frac{1}{\hbar^2}\frac{d^2E}{dK^2}\right)F$$

$$F = \left[\frac{\hbar^2}{\frac{d^2E}{dK^2}}\right] a = m^* a$$

$m^* \rightarrow$ "effective mass", in general not equal to the rest mass, and K-dependent!

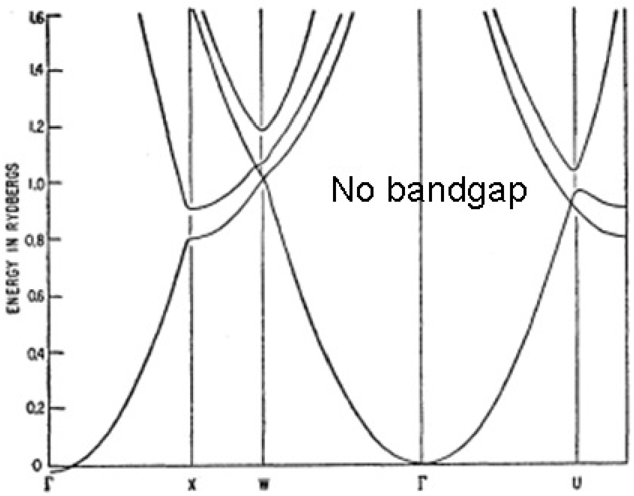
Trivial Example: plane wave $\quad E(K) = \frac{\hbar^2(K+g)^2}{2m}$

$$m^* = \frac{\hbar^2}{\frac{d^2E}{dK^2}} = \frac{\cancel{\hbar^2}}{\frac{d}{dK}\frac{\cancel{2}\cancel{\hbar^2}(K+g)}{\cancel{2}m}} = m$$

Effective masses are especially affected at bandgap edges...

The existence of bandgaps in the electron wave dispersion relation is critical to understanding why some crystals are metals and others are insulators or semiconductors. . . . Good Thing we have Quantum Mechanics!

Bandstructure Examples



← A metal (aluminum)

A semiconductor (silicon) →