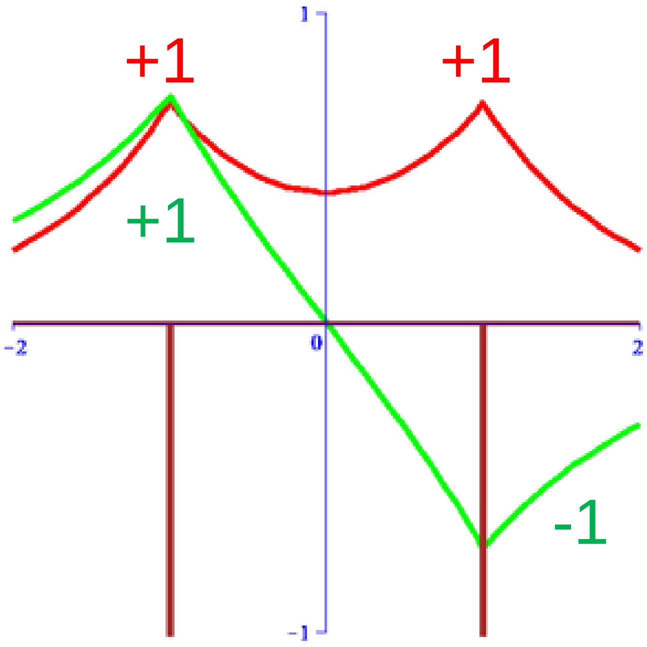
The two delta-functions discussed before correspond to q=0 and q=π.

This is because for N=2, the possible values of n=0,1,2, …, N-1 are just n = 0,1.



In the Dirac comb, in between the delta functions the potential is $V(x)=0$, and the solutions are simple [$(k\,\text{hbar})^2 = 2mE$]

$$\boxed{\psi(x) = A\sin(kx) + B\cos(kx), \quad (0 < x < a)}$$

Because we know the solution in the range $0<x<a$, then we know it everywhere, according to Bloch's theorem:

$$\boxed{\psi(x+a) = e^{iqa}\,\psi(x)}$$

This gives the wave function in the cell to the "right", if I have the wave function in the cell to the "left". Sometimes I have the wave function for the "right" cell, and I want the wave function for the "left cell": then use $\psi(x) = e^{-iqa}\,\psi(x+a)$.

$$\boxed{\psi(x) = e^{-iqa}\,\underbrace{[A\sin k(x+a) + B\cos k(x+a)]}_{\psi(x+a)}, \quad (-a < x < 0)}$$

To fix A and B, as with the delta function potential in QM P411, we will use:

(1) the wave function has to be continuous at x=0.
(2) the first derivative cannot be continuous for a delta function, but its discontinuity we know how to calculate.

Reminder: see again page 65 of the book for condition (2)

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\frac{d^2\psi}{dx^2}\,dx+\int_{-\epsilon}^{+\epsilon}V(x)\psi(x)\,dx=E\int_{-\epsilon}^{+\epsilon}\psi(x)\,dx$$

$$\Delta\left(\frac{d\psi}{dx}\right)\equiv\lim_{\epsilon\to0}\left(\left.\frac{d\psi}{dx}\right|_{+\epsilon}-\left.\frac{d\psi}{dx}\right|_{-\epsilon}\right)=\underbrace{\frac{2m}{\hbar^2}\lim_{\epsilon\to0}\int_{-\epsilon}^{+\epsilon}\underset{\Big\uparrow\,+\,\alpha\,\delta(x)}{V(x)}\psi(x)\,dx}_{=\frac{2m\alpha}{\hbar^2}\psi(0)}$$

(1) Continuity at x=0 requires that wave function

$$\psi(x) = A\sin(kx) + B\cos(kx), \quad (0 < x < a)$$

at x=0, i.e. $\psi(x=0) = B$, be equal to

$$\psi(x) = e^{-iqa}\,[A\sin k(x+a) + B\cos k(x+a)], \quad (-a < x < 0)$$

at x=0, which is $\psi(x=0) = e^{-iqa}\,[A\sin(ka) + B\cos(ka)]$

Thus, the first equation is:

$$\boxed{B = e^{-iqa}\,[A\sin(ka) + B\cos(ka)]}$$

q has to do with periodicity of the lattice; k has to do with the energy *E* *inside each cell*. Do not confuse them.

(2) The derivative of each of the two wave functions can be easily calculated and then specialized for x=0.

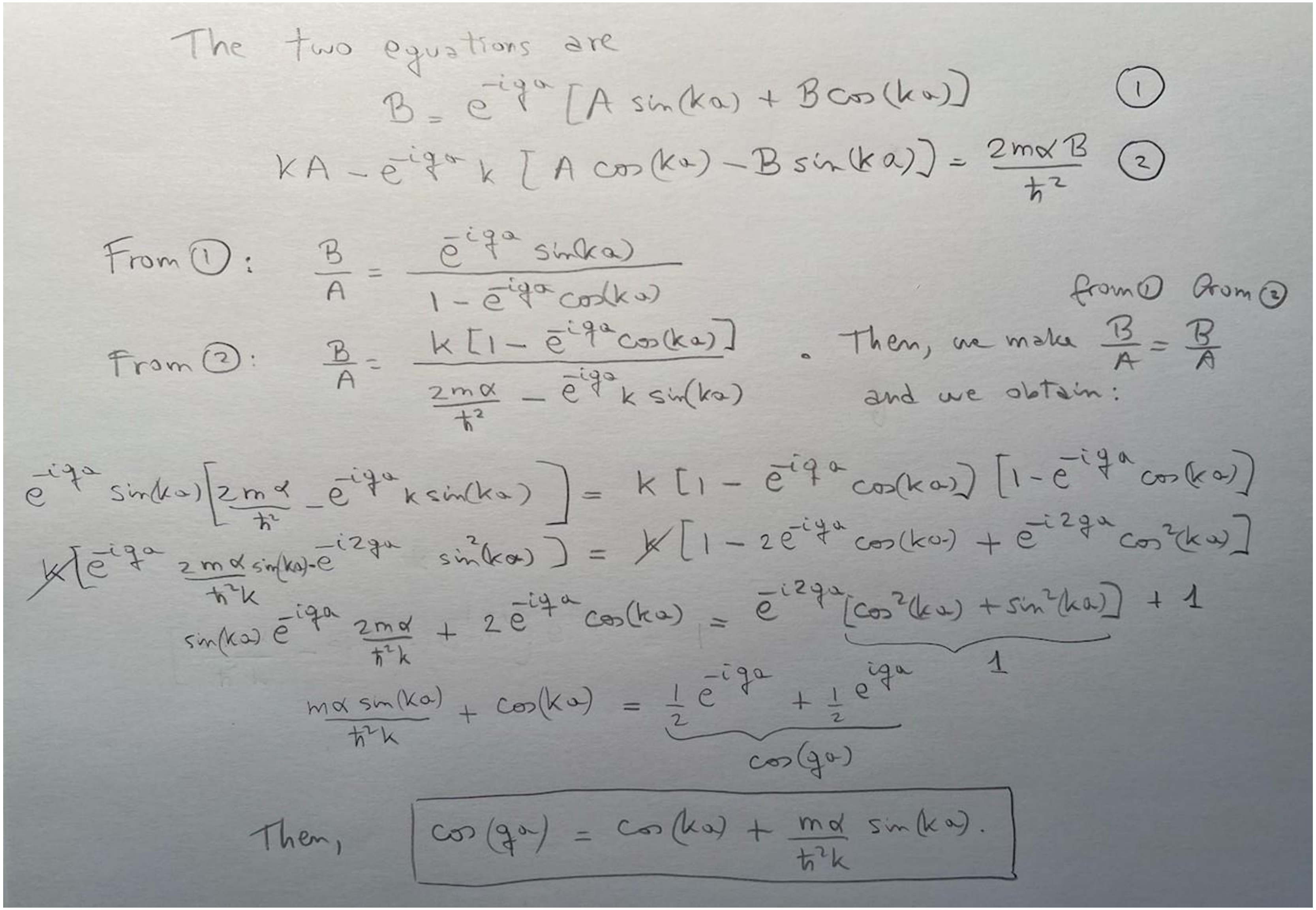
$$\boxed{kA - e^{-iqa}\, k[A\cos(ka) - B\sin(ka)] = \frac{2m\alpha}{\hbar^2}B}$$

$$\underbrace{\lim_{\epsilon\to 0}\left(\frac{d\psi}{dx}\bigg|_{+\epsilon} - \frac{d\psi}{dx}\bigg|_{-\epsilon}\right)}_{} \qquad \underbrace{= \frac{2m\alpha}{\hbar^2}\psi(0)}_{}$$

So, we have the two equations for A and B, easy to solve. There is no "independent" term i.e. each term has either A or B in front. Solving, leads to the condition that must be satisfied (derivation next page, just FYI):

$$\boxed{\cos(qa) = \cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka)}$$

Derivation of last formula of previous page, FYI



The two equations are

$$B = e^{-iqa}\left[A\sin(ka) + B\cos(ka)\right] \quad ①$$

$$kA - e^{-iqa}k\left[A\cos(ka) - B\sin(ka)\right] = \frac{2m\alpha B}{\hbar^2} \quad ②$$

From ①: $\dfrac{B}{A} = \dfrac{e^{-iqa}\sin(ka)}{1 - e^{-iqa}\cos(ka)}$

From ②: $\dfrac{B}{A} = \dfrac{k\left[1 - e^{-iqa}\cos(ka)\right]}{\dfrac{2m\alpha}{\hbar^2} - e^{-iqa}k\sin(ka)}$. Then, we make $\overset{\text{from ①}}{\dfrac{B}{A}} = \overset{\text{from ②}}{\dfrac{B}{A}}$ and we obtain:

$$e^{-iqa}\sin(ka)\left[\frac{2m\alpha}{\hbar^2} - e^{-iqa}k\sin(ka)\right] = k\left[1 - e^{-iqa}\cos(ka)\right]\left[1 - e^{-iqa}\cos(ka)\right]$$

$$\cancel{k}\left[e^{-iqa}\frac{2m\alpha}{\hbar^2 k}\sin(ka) - e^{-i2qa}\sin^2(ka)\right] = \cancel{k}\left[1 - 2e^{-iqa}\cos(ka) + e^{-i2qa}\cos^2(ka)\right]$$

$$\sin(ka)\,e^{-iqa}\frac{2m\alpha}{\hbar^2 k} + 2e^{-iqa}\cos(ka) = e^{-i2qa}\underbrace{\left[\cos^2(ka) + \sin^2(ka)\right]}_{1} + 1$$

$$\frac{m\alpha\sin(ka)}{\hbar^2 k} + \cos(ka) = \underbrace{\frac{1}{2}e^{-iqa} + \frac{1}{2}e^{iqa}}_{\cos(qa)}$$

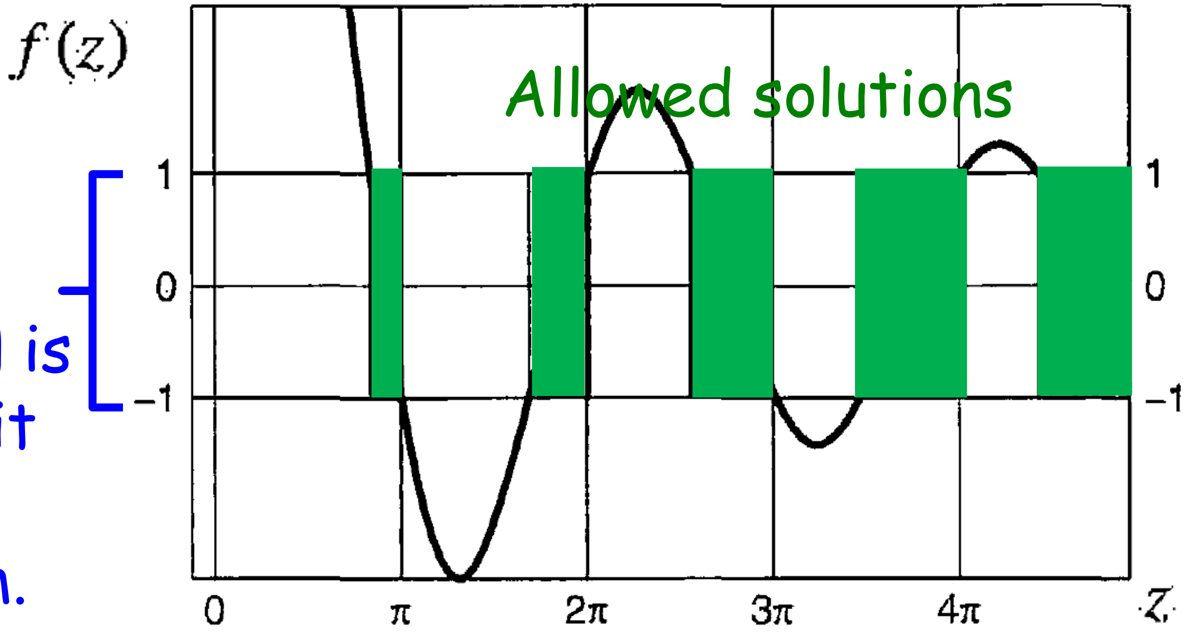
Then, $\boxed{\cos(qa) = \cos(ka) + \dfrac{m\alpha}{\hbar^2 k}\sin(ka).}$

Introducing: $z \equiv ka,$ and $\beta \equiv \frac{m\alpha a}{\hbar^2}$

then we arrive to:

$$\boxed{\underbrace{\cos(qa)}_{\text{Bounded between -1 and 1}} = \underbrace{\cos(z) + \beta\frac{\sin(z)}{z}}_{\text{Unbounded}}} = f(z)$$

Range of cos(*qa*). *qa*=2πn/N is so dense it forms a continuum.

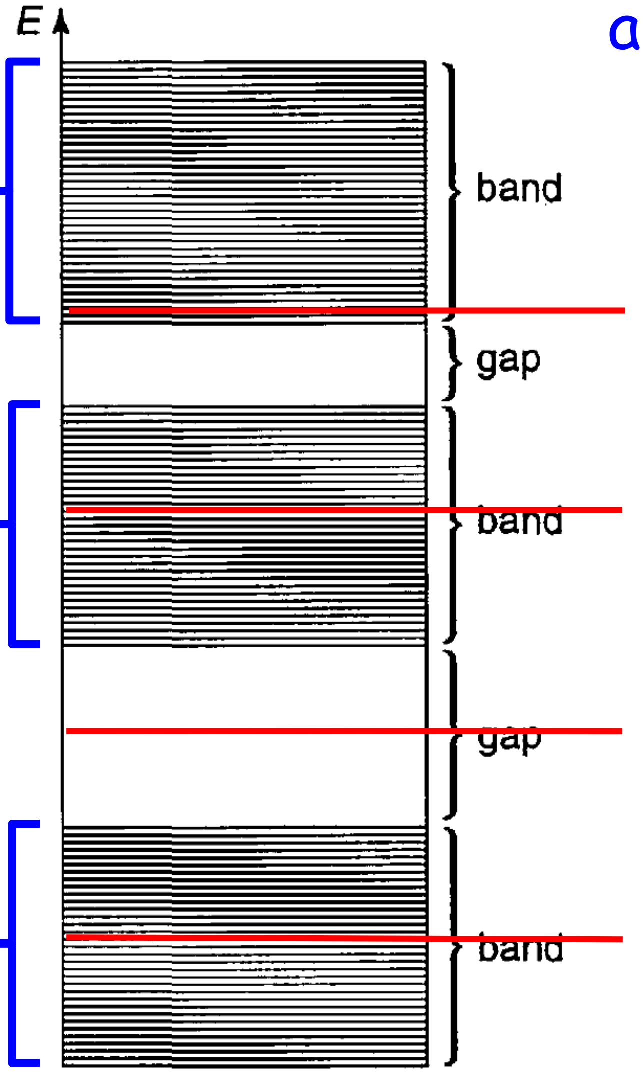


β = 10 as example

$$k \equiv \frac{\sqrt{2mE}}{\hbar}$$

Gaps and bands typically of width order eV

Repeating: $qa=2\pi n/N$ is so dense it forms almost a continuum.



N states

N states

N states (degenerate by pairs see HW problem, so N/2 actual lines at large N)

d=4+ε (semiconductor)-> second band fully occupied + a few more electrons (2e/state)

d=3 (metal)-> second band half occupied (2e/state)

d=2 (insulator)-> first band fully occupied (2e/state; line goes anywhere in gap)

d=1 (metal) -> half-band occupied (remember 2e/state; i.e. in the first N/2 states you can locate N electrons, and Nd=N for d=1)