What is the value of *q*? For this purpose I have to use another common trick: periodic boundary conditions.

Instead of a very long line of length ~ Na with N~ 10^{23} we will use a circle with the same perimeter. The physics cannot depend on this boundary effect.

$$\psi(x + Na) = \psi(x)$$

This trick fixes the value of *q* because

$$\psi(x + a) = e^{iqa}\,\psi(x) \longrightarrow \psi(x \underbrace{+\,a}_{N}) = \overbrace{e^{iqa}}^{N}\,\psi(x) = \psi(x)$$

$$\boxed{e^{iNqa}\,\psi(x) = \psi(x)}$$

If $e^{iNqa}\psi(x)=\psi(x)$, then $e^{iNqa}=1$ i.e. $Nqa=2\pi n$

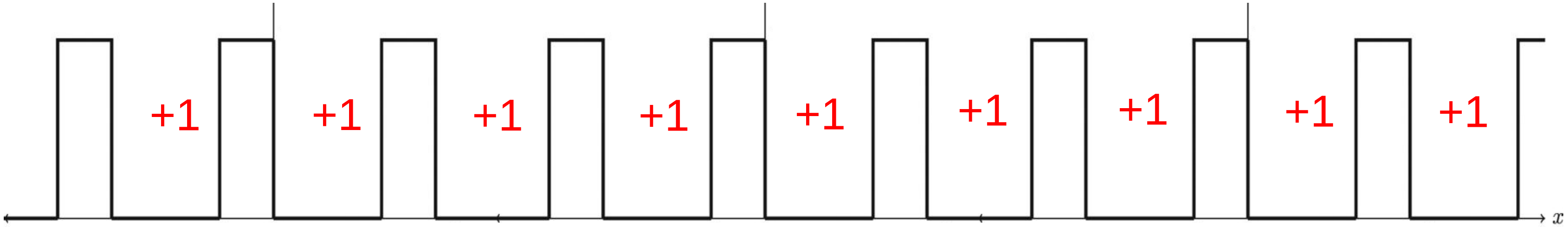
$$\boxed{q=\frac{2\pi n}{Na}, \quad (n=0,\ \pm 1,\ \pm 2,\ \ldots).}$$

Or n=0,1,2,…,N-1

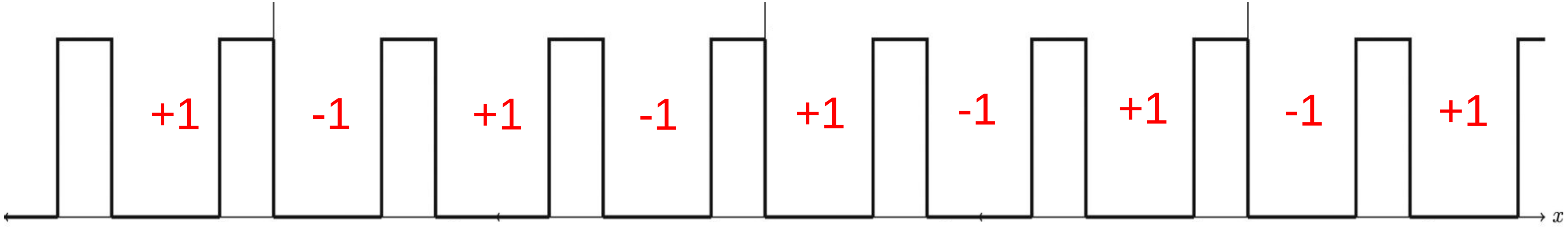
This theorem is independent of the “Dirac comb” we will use. It is valid for any periodic potential.

The importance is that you solve in the range 0<x<a, and then simply repeat the solution with different values of q, i.e. with different phase factors.

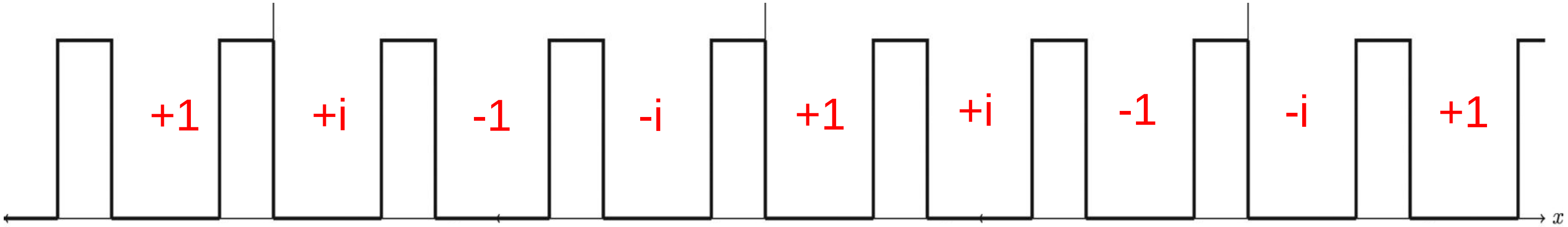
$qa=2\pi \times 0/N=0$



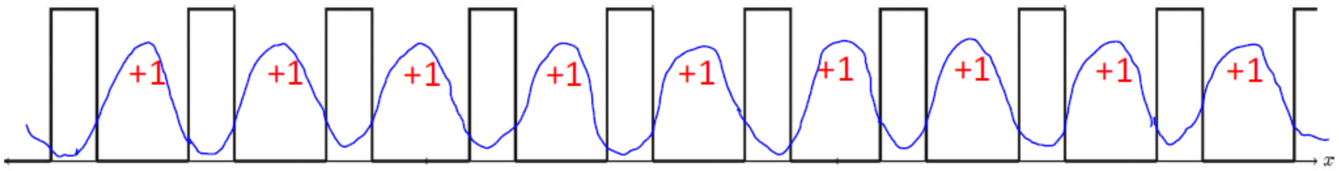
$qa=2\pi \times (N/2)/N= \pi$



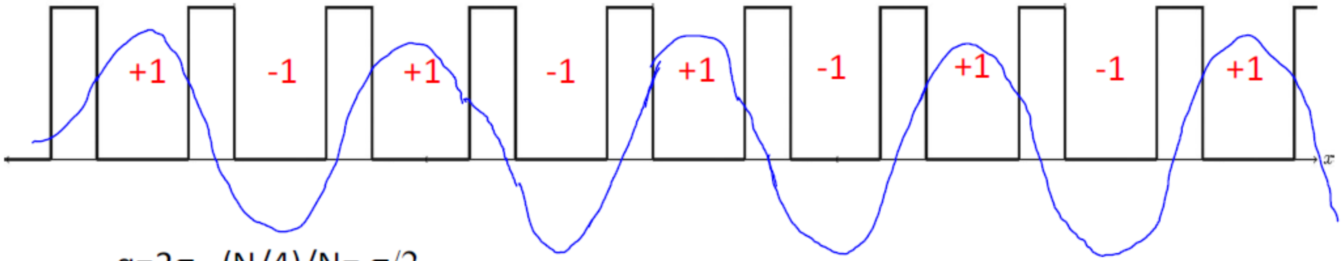
$qa=2\pi \times (N/4)/N= \pi/2$



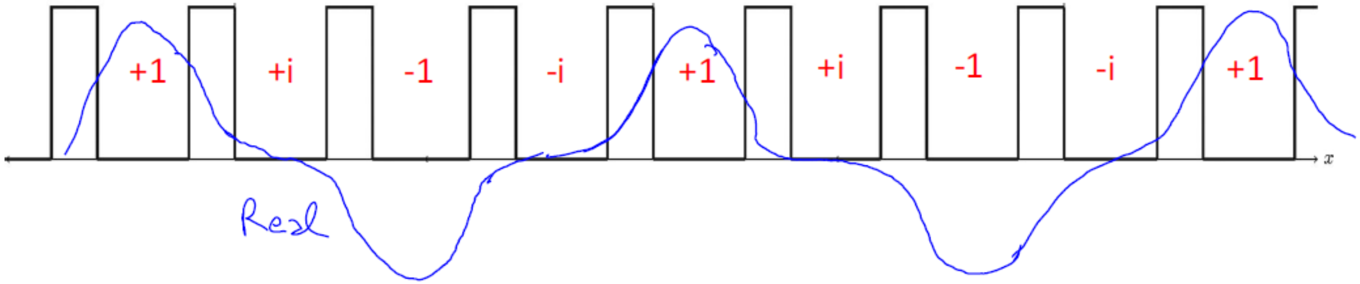
$q=2\pi \times 0/N=0$



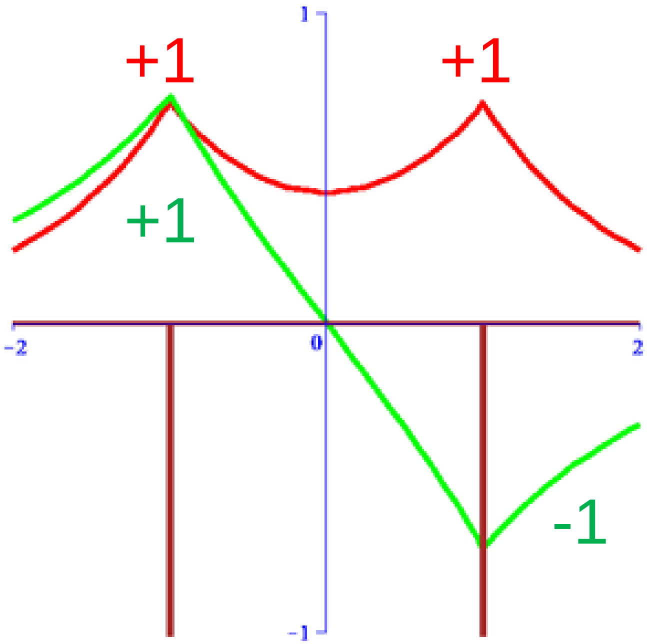
$q=2\pi \times (N/2)/N= \pi$



$q=2\pi \times (N/4)/N= \pi/2$



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



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

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

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 in the "right" cell, and I want the wave function in the "left cell": $\psi(x) = e^{-iqa}\,\psi(x+a)$.

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

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 page 65 of the book:

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

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

(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. Do not confuse them.

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

$$\boxed{\underbrace{kA - e^{-iqa}\, k[A\cos(ka) - B\sin(ka)]}_{\lim_{\epsilon\to 0}\left(\frac{d\psi}{dx}\Big|_{+\epsilon} - \frac{d\psi}{dx}\Big|_{-\epsilon}\right)} = \underbrace{\frac{2m\alpha}{\hbar^2}B}_{= \frac{2m\alpha}{\hbar^2}\psi(0)}}$$

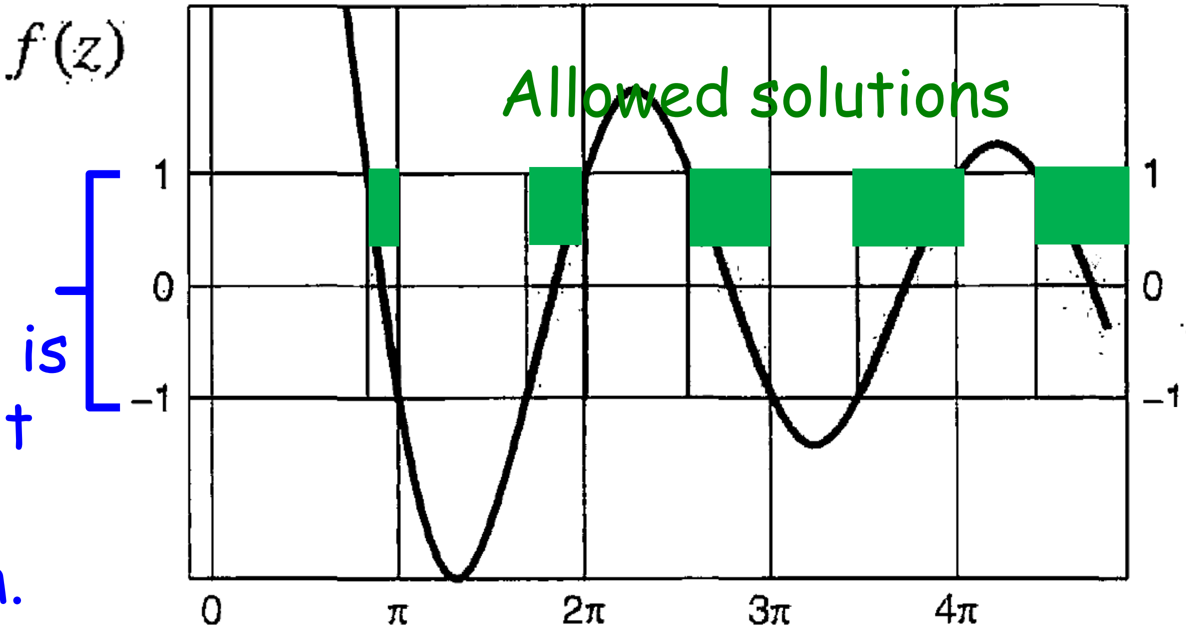
So, we have the two equations for A and B, easy to solve. There is no "independent" term i.e. each term has either *A* or *B* in front. Solving, leads to the condition that must be satisfied:

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

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.

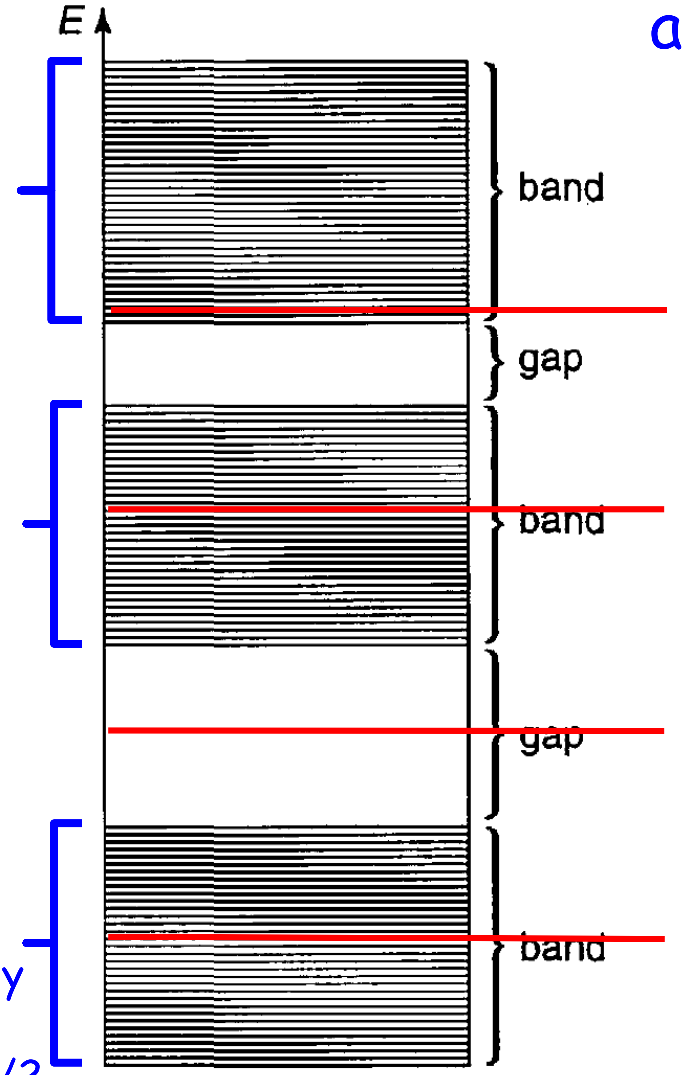
β = 10 as example

$z \equiv ka$

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

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)

d=1 (metal) -> half-band occupied (2e/state)