Periodic Potentials: Translational Symmetry

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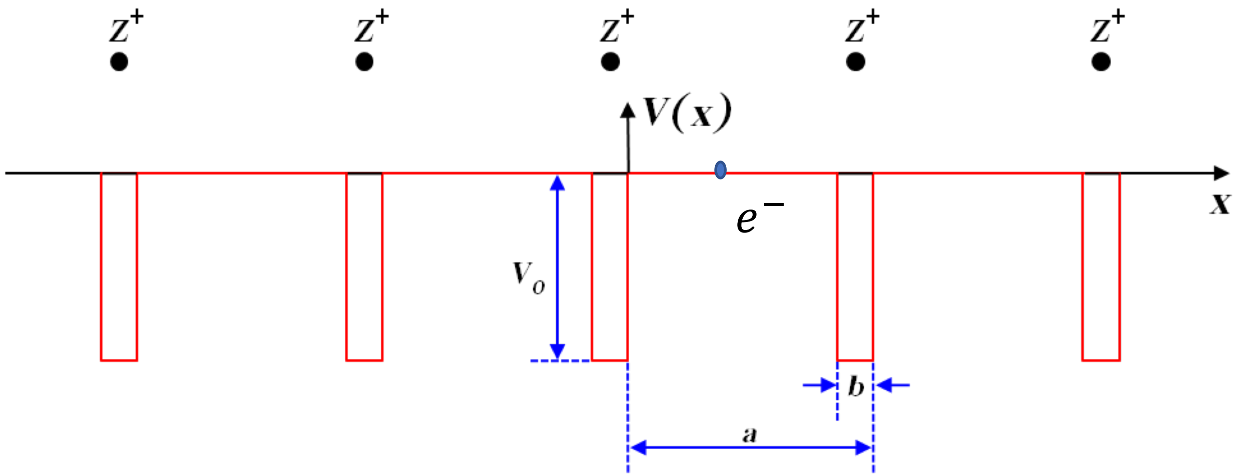
Goal: Understand set of problems featuring translational invariance that are likely to be on subject exam

- In class we looked at two classes of problems
    1. Translational invariant interaction (periodic potential problem like Kronig-Penny Model)
    2. Translationally invariant systems (circular chain of mass in notes)

- Typically, these problems involve solving for the energy levels of a particle (or many particles) in the presence of a periodic potential.

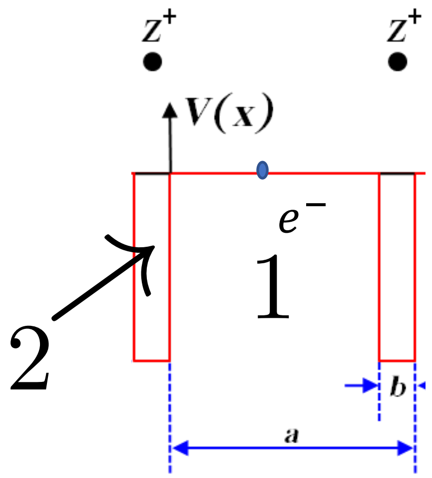
- I think for the subject exam, we would only need to worry about 1-d problems however, a lot of what we cover here can carry over to 2-d and 3-d. For example, it might be possible to reduce a 3-d or a 2-d problem to a 1-d problem.

Without getting too crazy, I think the Kronig-Penny model in 1-d has a lot of useful physics for the subject exam.



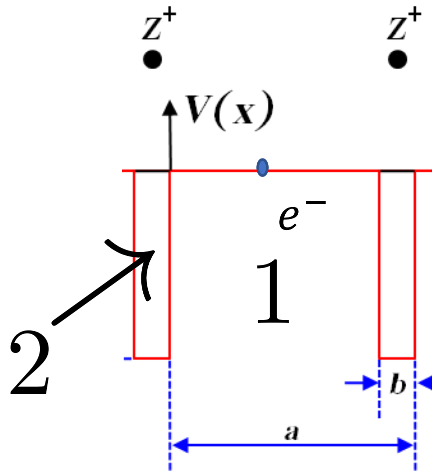
Problem: 1-d lattice with periodic step potentials. Find the allowed energy levels of an electron in this lattice.

- The first step in solving any periodic potential problem is to first ignore the lattice



Problem: 1-d lattice with periodic step potentials. Find the allowed energy levels of an electron in this lattice.

- The first step in solving any periodic potential problem is to first ignore the lattice.
- This is a much easier problem to solve. First we solve the Schrodinger equation in regions 1 and 2
- For now, we assume the electron's energy is $E > 0$



$\underline{0 < x < a - b}$ (Region 1)

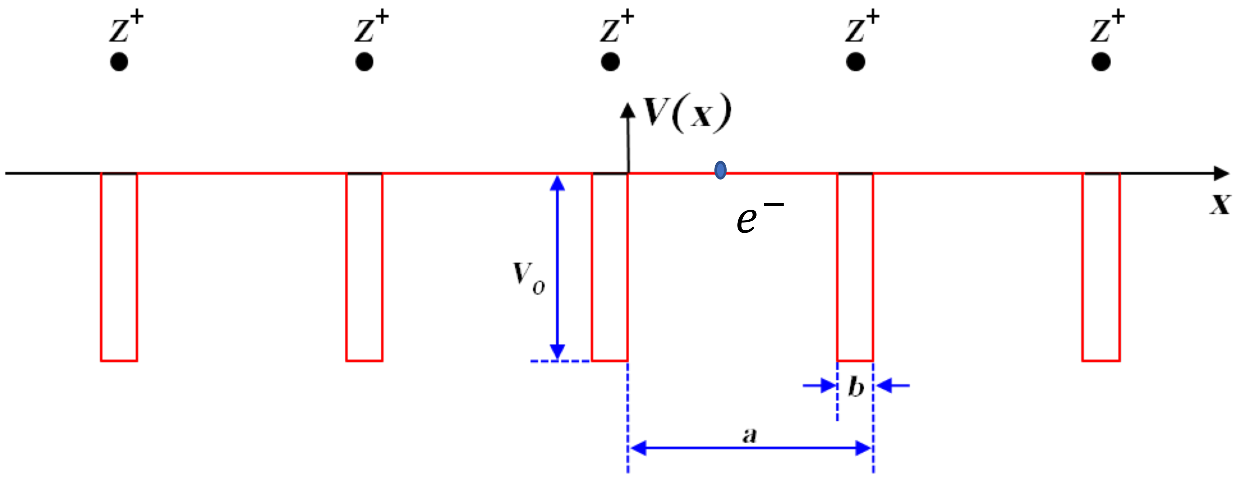
$$\frac{-\hbar^2}{2m}\psi''(x) = E\psi(x) \xrightarrow{\text{Solve}} \psi_1(x) = Ae^{i\alpha x} + Be^{-i\alpha x}$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}}$$

$\underline{-b < x < 0}$ (Region 2)

$$\frac{-\hbar^2}{2m}\psi_2''(x) = (E - V)\psi_2(x) \xrightarrow{\text{Solve}} \psi_2(x) = Ce^{i\beta x} + De^{-i\beta x}$$

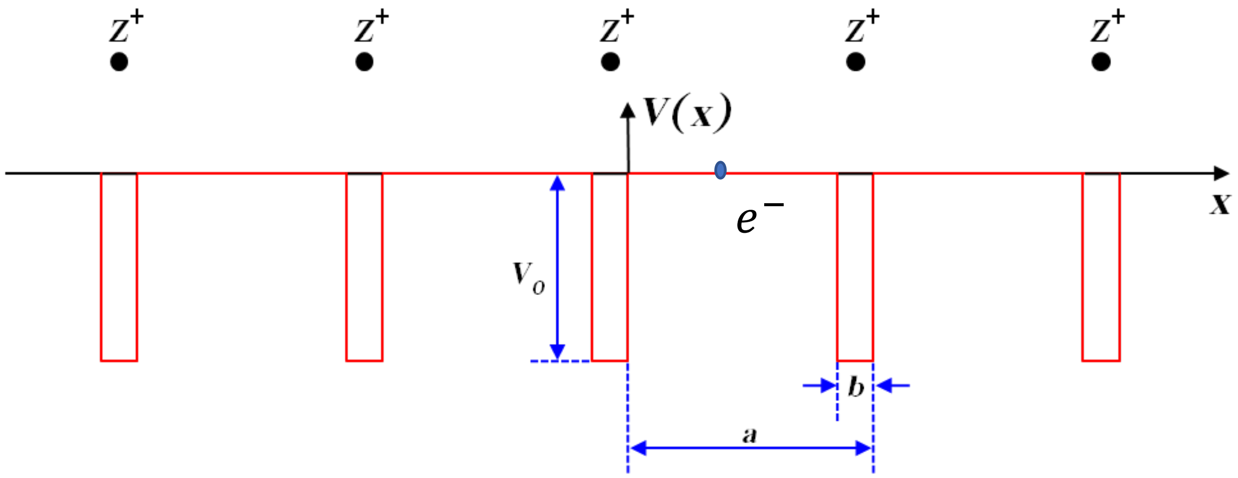
$$\beta = \sqrt{\frac{2m(E + V)}{\hbar^2}}$$



- Now that we have our solutions for simple problem, we need to extend it to a periodic lattice.
- We require that $\psi(x) = \psi(x + na)$ where n is an integer. This is known as a Born-Von Karman Boundary condition.
- Since our potential is periodic, $V(x) = V(x + na)$, the translational operator commutes with the Hamiltonian. This means our wavefunctions can be eigenfunctions of τ_a and H.
- Any time we have these two conditions, we can apply Bloch's Theorem (no proof here)

$$\psi(x) = e^{ikx}u(x)$$

Where $u(x)$ has the same periodicity as the lattice



- Now that we know the form of our solution, we now need to consider boundary conditions:

1. Continuity on both boundaries:

$$\psi_1(0) = \psi_2(0) \qquad \psi_1(a-b) = \psi_2(-b)$$

2. Smoothness on both boundaries:

$$\psi_1'(0) = \psi_2'(0) \qquad \psi_1'(-b) = \psi_2'(a-b)$$

- Skipping the algebra, we get 4 equations and 4 unknowns.

$$A + B = C + D$$

$$\alpha A - \alpha B = \beta C - \beta D$$

$$Ae^{i(\alpha-k)(a-b)} + Be^{-i(\alpha+k)(a-b)} = Ce^{-i(\beta-k)b} + De^{i(\beta+k)b}$$

$$A(\alpha-k)e^{i(\alpha-k)(a-b)} - B(\alpha+k)e^{-i(\alpha+k)(a-b)} = -(\beta-k)C(e^{-i(\beta-k)b} + D(\beta+k)e^{i(\beta+k)b}$$

$$\Big\downarrow$$

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ \alpha & -\alpha & -\beta & \beta \\ e^{i(\alpha-k)(a-b)} & e^{i(\alpha+k)(a-b)} & -e^{-i(\beta-k)b} & -e^{i(\beta+k)b} \\ (\alpha-k)e^{i(\alpha-k)(a-b)} & -(\alpha+k)e^{-i(\alpha+k)(a-b)} & -(\beta-k)e^{-i(\beta-k)b} & (\beta+k)e^{i(\beta+k)b} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = 0$$

- This is of the form $A\vec{x} = 0$ and since we want a non-trivial solution, A needs to be singular. We guarantee this by solving det(A) = 0.

Result for E > 0:

$$\cos(ka) = \cos(\beta b)\cos(\alpha(a-b)) + \frac{\alpha^2+\beta^2}{2\alpha\beta}\sin(\beta b)\sin(\alpha(a-b))$$

What does it mean?

- This gives us the relationship between the electron's wave vector k (related to it's momentum) and the energy inside and outside the potential barriers.
- Since $\cos(ka) \in [-1, 1]$, this places a restriction on α and β (hence E) .
- There will exist some region of E that will not satisfy this equation. These regions where there are no solutions in the k-E plane are called "band gaps".

Result for E < 0: $\alpha \to i\alpha$

$$\cos(ka) = \cos(\beta b)\cosh(\alpha(a-b)) - \frac{\alpha^2+\beta^2}{2\alpha\beta}\sin(\beta b)\sinh(\alpha(a-b))$$

Recover Dirac Delta model solution:

$$\cos(ka) = \cos(\beta b)\cos(\alpha(a-b)) + \frac{\alpha^2+\beta^2}{2\alpha\beta}\sin(\beta b)\sin(\alpha(a-b))$$

- To get the Dirac delta solution, we take $b \longrightarrow 0 \quad V_0 \longrightarrow \infty$

$$\cos(\beta b) \sim 1 \;\; \text{as} \;\; b \to 0$$

$$\sin(\beta b) \sim \beta b \;\; \text{as} \;\; b \to 0$$

$$\cos(ka) \sim \cos(\alpha a) + p\frac{\sin(\alpha a)}{\alpha} \;\; \text{as} \;\; b \to 0, V_0 \to \infty$$

$$p = \frac{mV_0 b}{\hbar^2}$$