

PH253 Lecture 15: Schrödinger's equation. Still. 1-D potentials

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Image of the day

High-resolution electron microscope image of a $\text{Co}_{1.5}\text{Ti}_{0.5}\text{FeGe}$ alloy sample. The bright dots are individual atoms. The inset is a Fourier transform of the image, indicating the hexagonal symmetry.

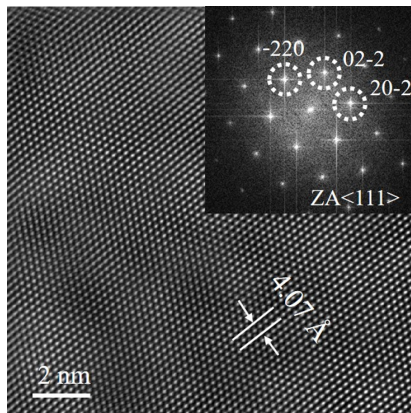


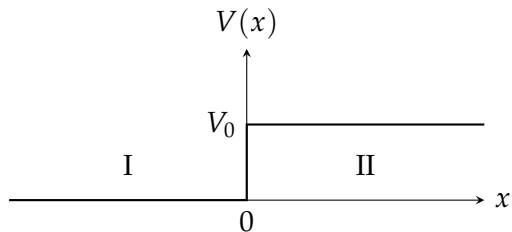
Figure: UA Physics / LeClair group / Phys. Rev. Materials 3, 114406 (2019)

Outline

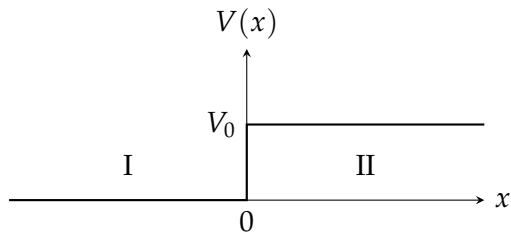
- 1 Potential step
- 2 Particle in a box
- 3 Observables and operators



Potential step from last time



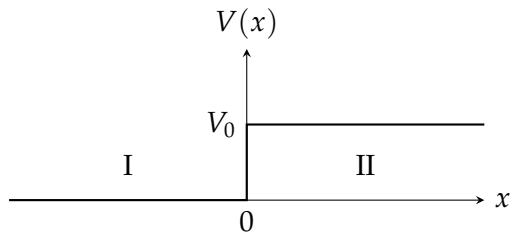
Potential step from last time



$$\psi(x)_I = e^{ikx} + Re^{-ikx} \quad \psi(x)_{II} = Te^{iqx}$$

$$R = \frac{k - q}{k + q} \quad T = \frac{2k}{k + q} \quad k^2 = \frac{2mE}{\hbar^2} \quad q^2 = \frac{2m(E - V_0)}{\hbar^2}$$

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Transmission is highly energy-dependent

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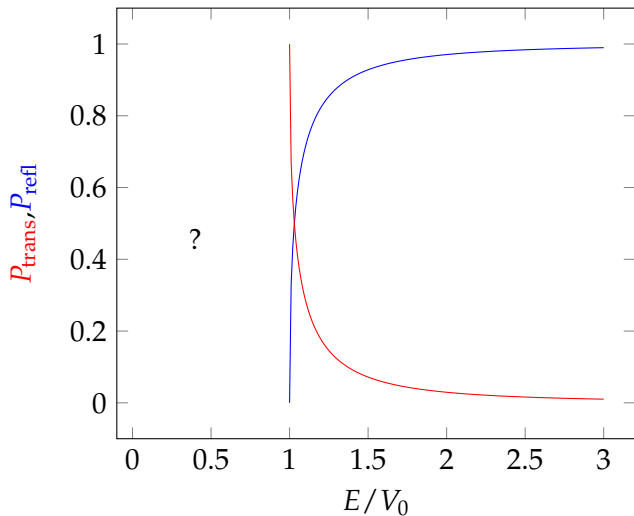
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- 6 $E = V_0$? $P_{\text{trans}} = 0$, perfect reflection



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Some interesting aspects

- 1 Classical: go over step, slow down to conserve E , never reflect



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$$\psi_{II} = T e^{-|q|x} \quad T = \frac{2k}{k + i|q|} \neq 0 \quad (E < V_0)$$



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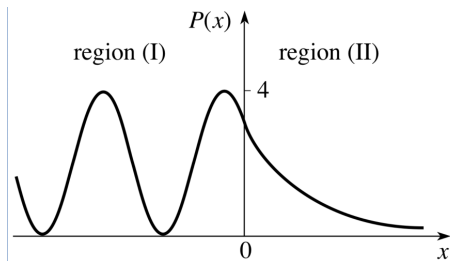


Figure: http://www.met.reading.ac.uk/pplato2/h-flap/phys11_1.html



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Particle in a box

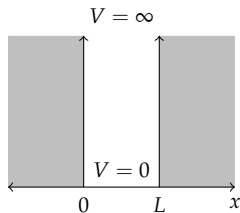
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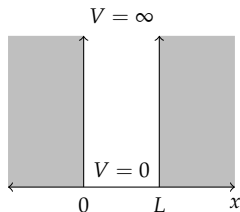
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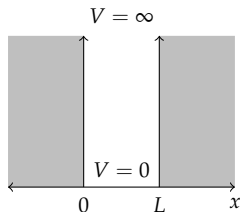
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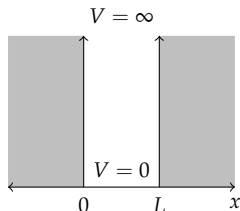
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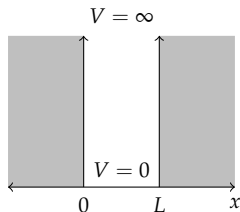
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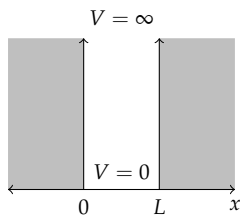


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- 5 Implies boundary condition $\psi(0) = \psi(L) = 0!$

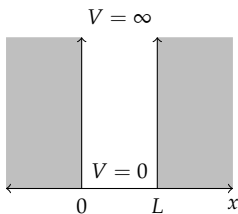


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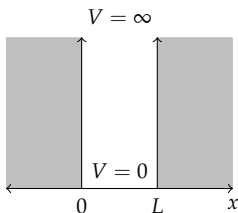
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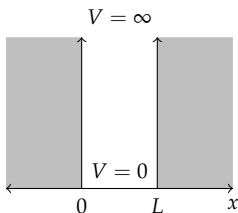
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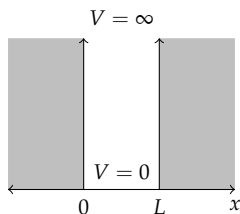
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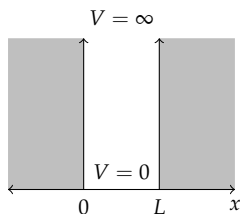


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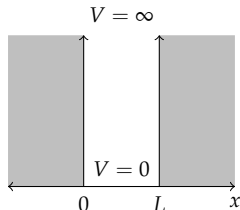
Now set up Schrödinger's equation in box + boundary conditions.



Boundary conditions are key

Schrödinger equation with $V = 0$:

$$\frac{d^2\psi}{dx^2} = -\left(\frac{2mE}{\hbar^2}\right)\psi = -k^2\psi \quad \left(\text{with } k^2 = \frac{2mE}{\hbar^2}\right)$$

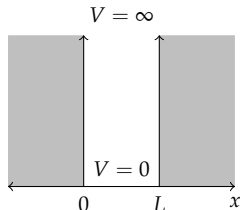


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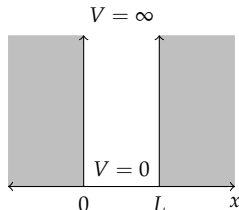
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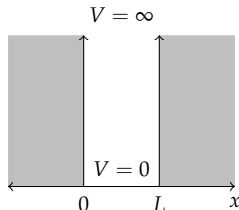
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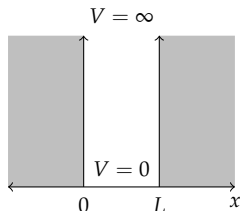
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How to find constants? Boundary conditions! $\psi(0) = \psi(L) = 0$



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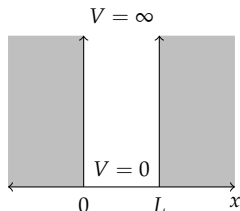


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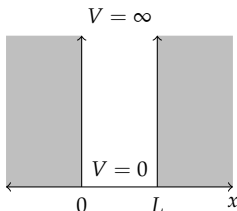
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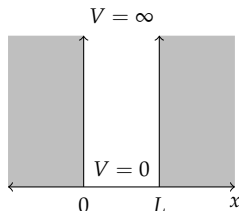
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Recall: bound states have ψ purely real



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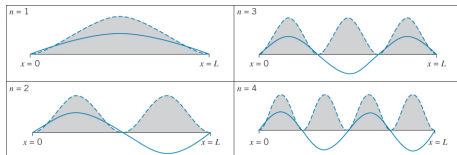


Figure: Krane, *Modern Physics*. Solid: ψ . Dashed: $|\psi|^2$.

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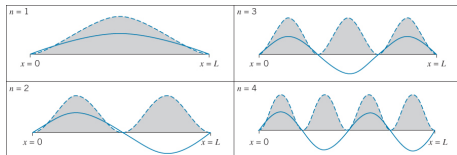


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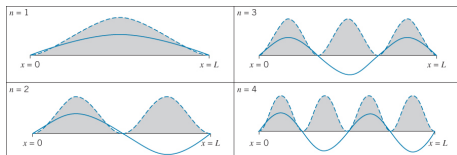


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$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} = \frac{n^2 h^2}{8mL^2}$$

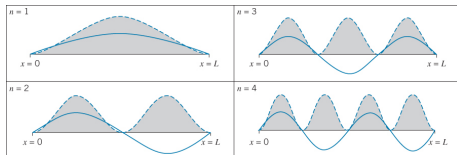


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$$\psi(x) = \begin{cases} C_n \sin\left(\frac{n\pi x}{L}\right) & 0 \leq x \leq L \\ 0 & x < 0, x > L \end{cases}$$

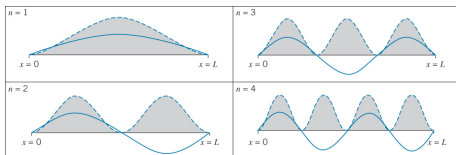


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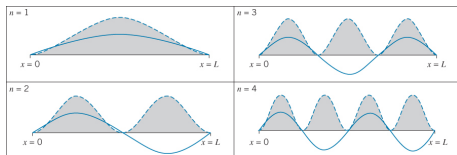


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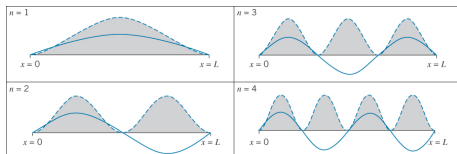


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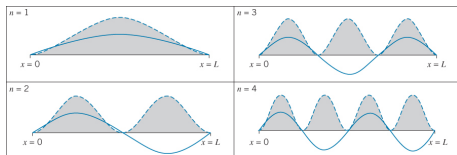


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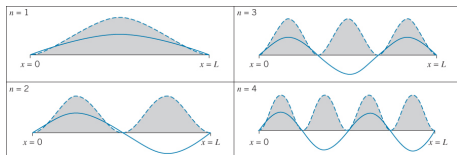


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- 3 Integrand only nonzero from 0 to L though!



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$$\psi(x) = \begin{cases} C_n \sin\left(\frac{n\pi x}{L}\right) & 0 \leq x \leq L \\ 0 & x < 0, x > L \end{cases}$$

- 1 What are the C_n ? We have not normalized the wave function ...
- 2 Enforce $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$
- 3 Integrand only nonzero from 0 to L though!

$$\begin{aligned} 1 &= \int_0^L |\psi(x)|^2 dx = \int_0^L C_n^2 \sin^2\left(\frac{n\pi x}{L}\right) dx \\ &= C_n^2 \left[\frac{x}{2} - \frac{4L}{n\pi} \sin\left(2\frac{n\pi x}{L}\right) \right] \Big|_0^L = C_n^2 \frac{L}{2} \end{aligned}$$



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- 8 What about position, and how to use these new operators?



Outline

- 1 Potential step
- 2 Particle in a box
- 3 Observables and operators



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$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^* x \psi dx = \int_{-\infty}^{+\infty} x |\psi(x)|^2 dx = \int_{-\infty}^{+\infty} x P(x), dx$$



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$$1 = \int_{-\infty}^{+\infty} P(x), dx$$

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But! Can now formalize uncertainty principle & actually calculate.



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- ③ Measurement? $x_{\text{best}} = \langle x \rangle \pm \langle x^2 \rangle = (0.500 \pm 0.289)L$ – broad



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- 3 We know $p^2 = 2mE$ for a free particle, must be true in box too ...



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- 3 Not unreasonable: uncertainty up as n (and E_n) increase



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- 6 Up next: modeling atoms

