Ordinary Differential Equations

- Eigenvalue problems.
- Shooting method.
- Numerov's method.

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  - Every term is linear in the dependent variable.
- A good example is the Schrödinger equation:

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

where the symbols have the usual meaning.

Eigenvalue problems

- Consider the problem of a particle in a square potential well of length L with infinitely high walls, i.e.

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- As the probability of finding the particle in the region with $V(x) = \infty$ is zero, the wavefunction $\psi(x)$ has to go to zero at $x = 0$ and $x = L$.
- Standard boundary value problem, that we can solve with the Shooting method!

- As this is a second order differential equation, we would start by turning it into 2 first order differential equations:

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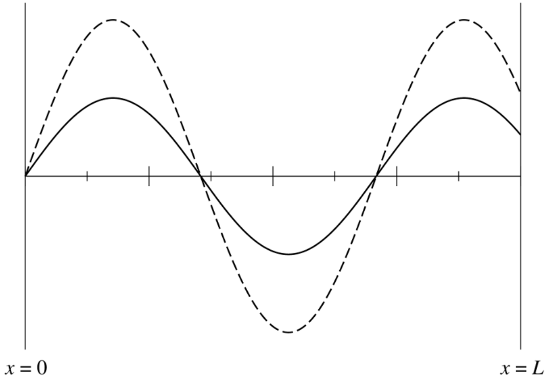
- We know $\psi(x = 0) = 0$. We guess an initial value of ϕ and then calculate the solution from $x = 0$ to $x = L$ (using for example 4th order Runge Kutta).

Shooting method

- We see that the solution does not go to 0 at $x = L$.



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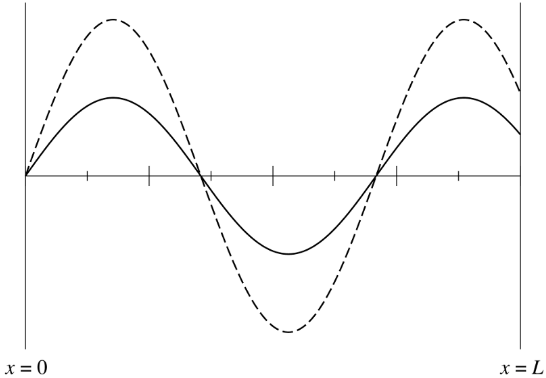
- We can try to fix this by changing the initial condition on ϕ using a root finding method (such as binary search).



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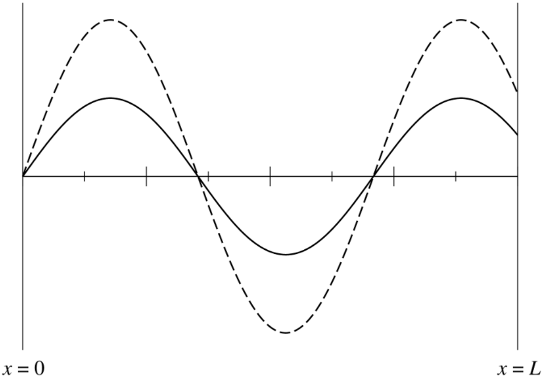

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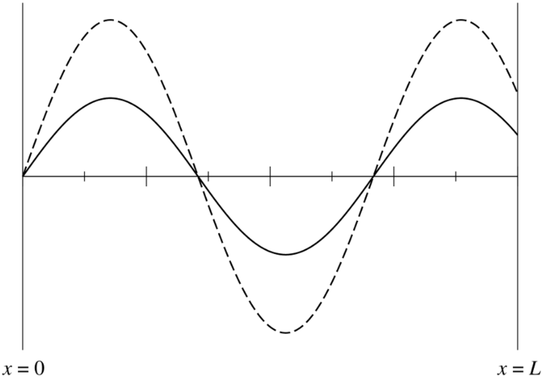
- If we just double the initial condition on ϕ we get the dashed curve!



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- This is because the equation is linear – if $\psi(x)$ is a solution, $c\psi(x)$ is also a solution!
- Infact for an arbitrary choice of E, there is no solution that satisfies the boundary conditions!
- The solutions exists only for some specific/allowed values of E – eigenvalues.

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- Since changing this boundary condition, only changes the solution by a simple multiplicative factor, it doesn't matter what this is set to!!!!
- Usually the factor is fixed by normalization of the wavefunction.

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- Instead of solving two first order differential equations solve the second order differential equation directly.
- Use the fact that this equation is linear in ψ and there is no term involving the first derivative.
- Let us rewrite the equation as:

$$\frac{d^2\psi}{dx^2} + k^2(x)\psi(x) = 0$$

where $k^2 = \frac{2m}{\hbar^2}(E - V(x))$

Numerov's method

Taylor expanding $\psi(x+h)$:

$$\psi(x+h) = \psi(x) + h\psi' + \frac{h^2}{2}\psi^{(2)} + \frac{h^3}{6}\psi^{(3)} + \frac{h^4}{24}\psi^{(4)} + \ldots$$

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Adding the Taylor expansion of $\psi(x-h)$:

$$\psi(x+h) + \psi(x-h) = 2\psi(x) + h^2\psi^{(2)} + \frac{h^4}{12}\psi^{(4)} + \mathcal{O}(h^6)\dots$$

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Rearranging terms we get:

$$\psi^{(2)} = \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{(4)} + \mathcal{O}(h^6)$$

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Substituting for $\psi^{(2)} + \frac{h^2}{12}\psi^{(4)}$:

$$\psi(x+h)+\psi(x-h)-2\psi(x)+h^2k^2(x)\psi(x)+\frac{h^4}{12}\frac{d^2}{dx^2}[k^2(x)\psi(x)] = 0$$

Using a simple central differencing formula ($\mathcal{O}(h^2)$) as it is already multiplied by h^4:

$$\frac{d^2}{dx^2}[k^2(x)\psi(x)] \approx \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2}$$

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Substituting and rearranging:

$$\psi(x{+}h) = \frac{2(1 - \frac{5}{12}h^2k^2(x))\psi(x) - (1 + \frac{1}{12}h^2k^2(x-h))\psi(x-h)}{1 + \frac{1}{12}h^2k^(x+h)}$$

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This method has error of $\mathcal{O}(h^6)$ per step.

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- There maybe problems in the subtraction in the numerator – so only use double/double precision.