5) Further Applications of Schroedinger's equation

Time dependence of quantum states

Stationary states satisfy the time independent Schrödinger equation.

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Phi(x)+V(x)\Phi(x)=E\,\Phi(x)$$

$$\Psi(x,t)=\Phi_n(x)e^{-i\frac{E_n}{\hbar}t} \quad \Rightarrow$$

The probability distribution is constant in time:

$$|\Psi|^2=|\Phi(x)|^2$$

and can therefore not describe moving particles

A linear combination of stationary states satisfies the time dependent Schrödinger equation and leads to time dependent probability distributions:

$$\Psi(x,t)=\Phi_n(x)e^{-i\frac{E_n}{\hbar}t}+\Phi_m(x)e^{-i\frac{E_m}{\hbar}t}$$

$$\begin{aligned}|\Psi|^2 &= (\Phi_n^* e^{i\frac{E_n}{\hbar}t}+\Phi_m^* e^{i\frac{E_m}{\hbar}t})(\Phi_n e^{-i\frac{E_n}{\hbar}t}+\Phi_m e^{-i\frac{E_m}{\hbar}t})\\ &=|\Phi_n|^2+|\Phi_m|^2+(\Phi_n^*\Phi_m e^{i\frac{E_n-E_m}{\hbar}t}+C.C.)\\ &=|\Phi_n|^2+|\Phi_m|^2+2\,\mathrm{Re}[\Phi_n^*\Phi_m e^{i\frac{E_n-E_m}{\hbar}t}]\end{aligned}$$

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Time dependent states in an infinite well

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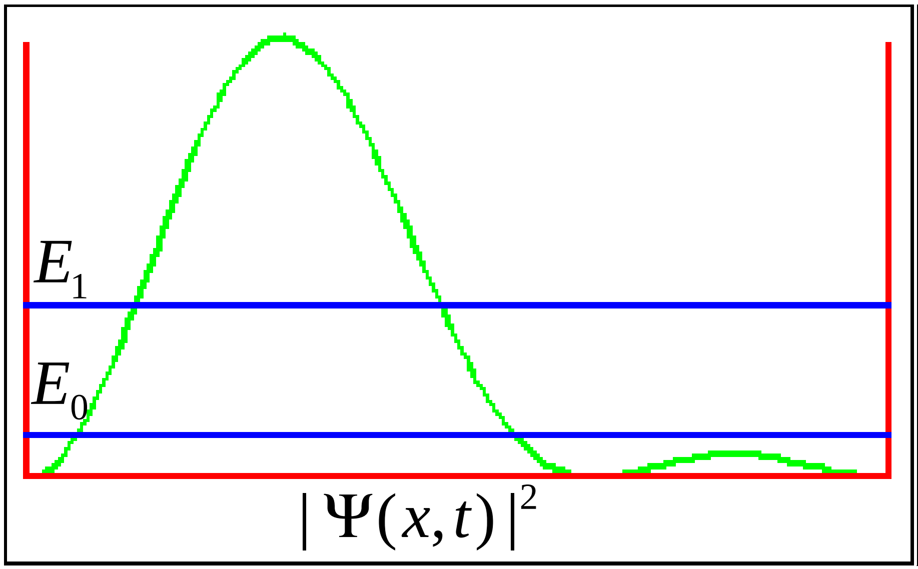
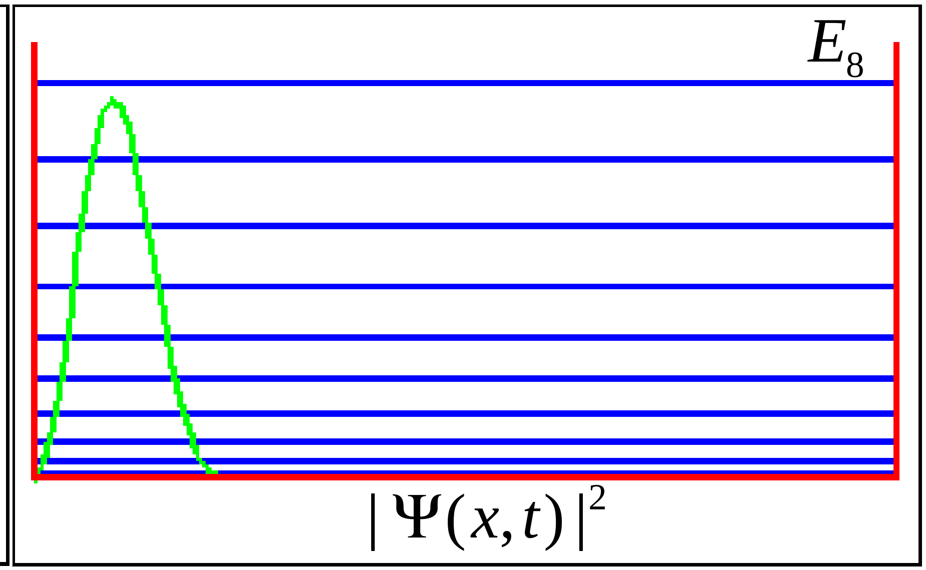
$$\Psi(x,t) \propto \Phi_0(x)e^{-i\frac{E_0}{\hbar}t} + A_1\Phi_1(x)e^{-i\frac{E_1}{\hbar}t} \qquad \Psi(x,t) = \sum_{n=0}^{8} A_n\Phi_n(x)e^{-i\frac{E_n}{\hbar}t}$$





Solutions of the time dependent Schrödinger equation can describe probability distributions that change with time and can describe traveling particles.

The **time average**, however, is only given by solutions of the time independent Schrödinger equation.

$$\left\langle |\Psi|^2 \right\rangle_t = \left\langle |\Phi_n|^2 + |\Phi_m|^2 + 2\,\mathrm{Re}[\Phi_n^*\Phi_m e^{i\frac{E_n - E_m}{\hbar}t}] \right\rangle_t = |\Phi_n|^2 + |\Phi_m|^2$$

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Orthogonality for stationary states of the infinite well

$$\Phi_n(x) = \sqrt{\tfrac{2}{L}}\sin([n+1]\tfrac{\pi}{L}x)e^{i\vartheta} \quad \rightarrow \quad \int_0^L |\Phi_n|^2\, dx = 1$$

$$\int_0^L \sin(n\tfrac{\pi}{L}x)\sin(m\tfrac{\pi}{L}x)dx = \tfrac{L}{\pi}\int_0^\pi \sin(n\xi)\sin(m\xi)d\xi$$

$$\propto \int_0^\pi (e^{in\xi} - e^{-in\xi})(e^{im\xi} - e^{-im\xi})d\xi$$

$$\propto \mathrm{Re}\{\int_0^\pi [e^{i(n-m)\xi} - e^{i(n+m)\xi}]d\xi\} = 0 \quad \text{for } n \neq m$$

$$\int_0^L \Phi_n^*(x)\Phi_m(x)\,dx = \delta_{nm} = \begin{cases} 1 \text{ if } n = m \\ 0 \quad \text{else} \end{cases}$$

The decomposition of functions in terms of sin and cos oscillations is also complete for a very large set of functions (all well behaved functions), i.e. an expansion can be found for all functions of this set.

Such an expansion is called a Fourier series.

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Initial value problems

Given: $\Psi(x,0) = f(x)$, what will be the time dependent wave function?

Find the expansion $f(x) = \sum_{n=0}^{N} A_n \Phi_n(x)$

The time dependent solution is then

$$\Psi(x,t) = \sum_{n=0}^{N} A_n \Phi_n(x) e^{-i\frac{E_n}{\hbar}t}$$

How can the coefficients A_n be found?

If the wave functions are orthogonal: $\int_{-\infty}^{\infty} \Phi_n^*(x)\Phi_m(x)\,dx = \delta_{nm} = \begin{cases} 1 \text{ if } n = m \\ 0 \quad \text{else} \end{cases}$

the coefficients can be found by projection:

$$A_n = \int_{-\infty}^{\infty} \Phi_n^*(x) f(x) dx$$

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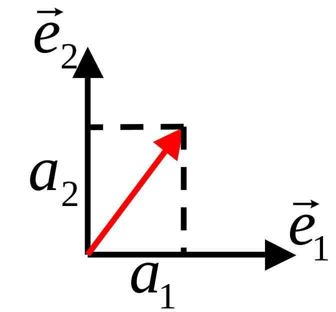
Initial value problems

Completeness:

There is an expansion $f(x) = \sum_{n=0}^{N} A_n \Phi_n(x)$

similar to $\vec{g} = \sum_{n=0}^{3} a_n \vec{e}_n$

How can the coefficients A_n be found?



Ortho-normality: $\int_{-\infty}^{\infty} \Phi_n^*(x)\Phi_m(x)\,dx = \delta_{nm} = \begin{cases} 1 \text{ if } n = m \\ 0 \quad \text{else} \end{cases}$

similar to $\vec{e}_n \cdot \vec{e}_m = \delta_{nm}$

The coefficients can be found by projection:

$$A_n = \int_{-\infty}^{\infty} \Phi_n^*(x) f(x) dx$$

similar to $a_n = \vec{e}_n \cdot \vec{g}$

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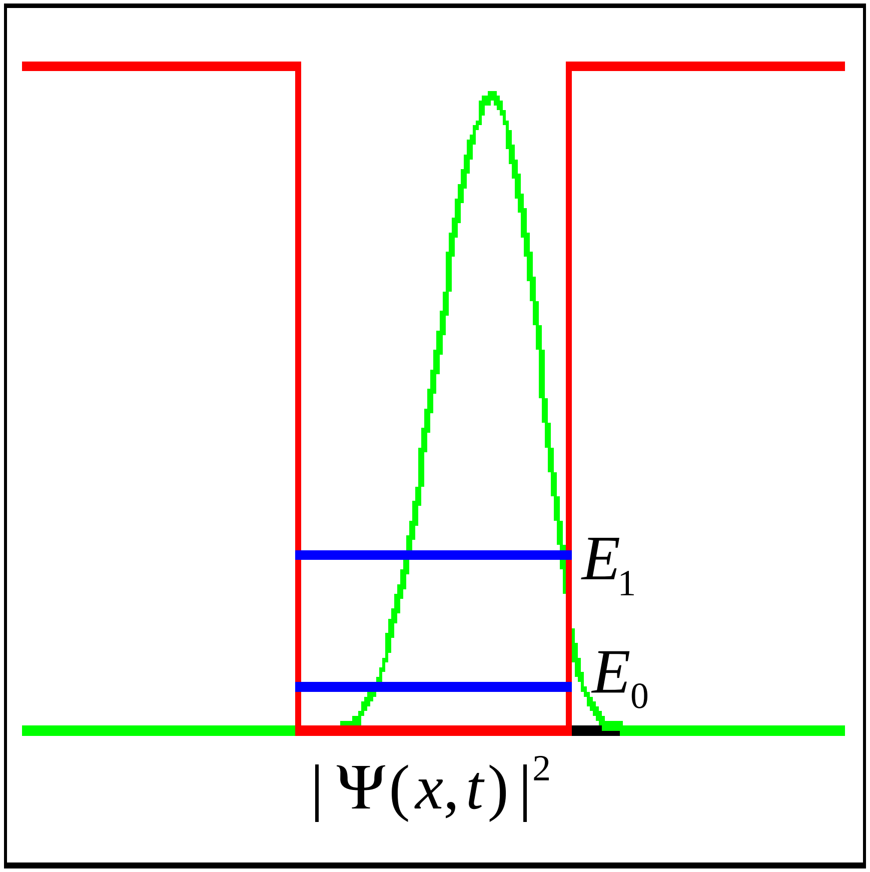
Time dependent states in a finite well

03/04/2005

$$\Psi(x,t) \propto \Phi_0(x)e^{-i\frac{E_0}{\hbar}t} + \tfrac{3}{4}\Phi_1(x)e^{-i\frac{E_1}{\hbar}t}$$



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Time dependent states in a finite well

$$\Psi(x,t) \propto \Phi_0(x)e^{-i\frac{E_0}{\hbar}t} + \tfrac{3}{4}\Phi_1(x)e^{-i\frac{E_1}{\hbar}t} \quad \Psi(x,t) \propto \Phi_0(x)e^{-i\frac{E_0}{\hbar}t} + \tfrac{3}{2}\Phi_2(x)e^{-i\frac{E_2}{\hbar}t}$$