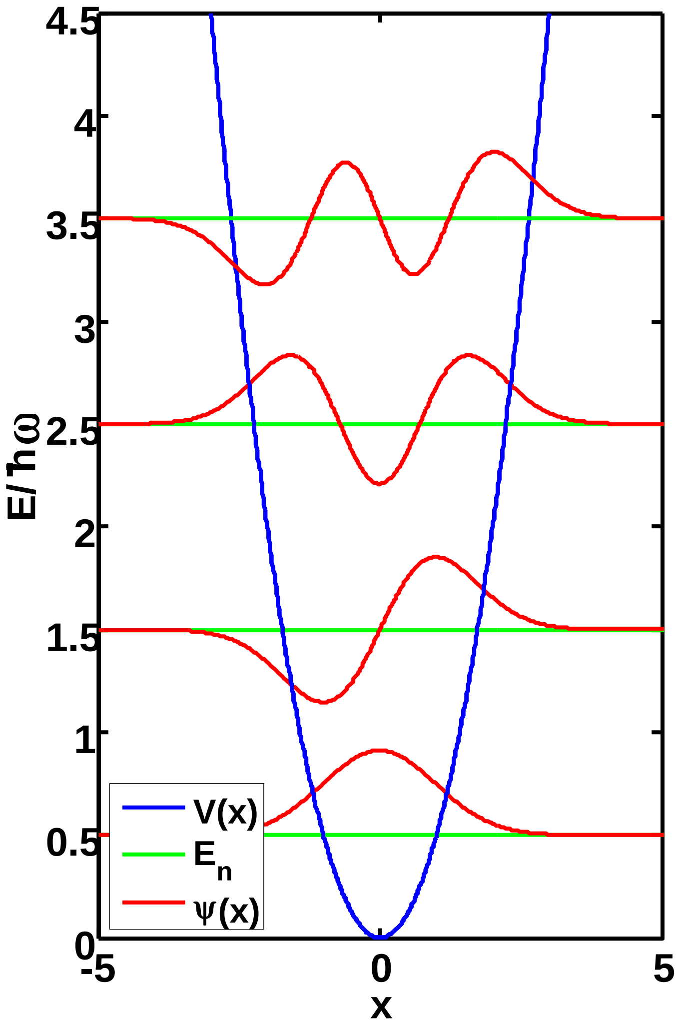
## Lecture 21: 03/09/09

- Superposition of stationary bound states
- Formalism I
  - Hilbert space and wavefunctions
  - Observables and hermitian operators

Recap:

## $II_{2,5}$ The simple harmonic oscillator potential $V(x)=1/2cx^2$:

$$V(x) = \frac{1}{2} c x^2 = \frac{1}{2} m \omega^2 x^2$$




$$\psi(\xi) = \sum_{j=0}^{\infty} a_j \xi^j e^{-\xi^2/2} \quad \text{solves S.E.}$$

$$\text{with} \quad a_{j+2} = \frac{2j+1-K}{(j+2)(j+1)} a_j$$

But: need to terminate power series to make $\psi(\xi)$ normalizable!

$$\Rightarrow a_{j+2} = \frac{2(j-n)}{(j+2)(j+1)} a_j$$

$$\psi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n \cdot n!}} H_n(\xi) e^{-\xi^2/2}$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, 3, \ldots$$

## Recap II:

## $II_{2,6}$ Numerical Solution of the time-indep. Schrödinger Equ.:

for most physically realistic potentials the S.E. cannot be solved in analytical form!

→ Solution: use numerical approximation methodes on computer!

Approximate difference Equation:

$$\boxed{\psi_{j+1} = \left\{ 2 - \Delta\bar{x}^2 \left[ \bar{E} - \bar{V}_j \right] \right\} \psi_j - \psi_{j-1}}$$

→ compute values of $\psi(\bar{x})$ only at certain, discrete, equally spaced values along the coordinate $\bar{x}$

$$\bar{x}_j = j \cdot \overbrace{\Delta\bar{x}}^{\text{grid spacing}}$$

$$\psi(\bar{x}_j) \equiv \psi_j$$

$$\bar{V}(\bar{x}_j) = \bar{V}_j$$

# III Formalism

1) Superposition of stationary bound states

2) Formalism: Hilbert space, observables,
eigenfunctions, ...

3) Polarization states of photons

⇒ "state vector"

⇒ projections

⇒ basis states

## III$_1$ Superposition of stationary, bound states:

given potential well: $V(x)$ with only bound states

$\Rightarrow$ need to solve the time-dep. Schrödinger Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\,\Psi(x,t) = \hat{H}\Psi$$

$\Rightarrow$ subset of solutions: stationary bound states:

$$\Psi_n(x,t) = \psi_n(x)\, e^{-iE_n/\hbar \cdot t}$$

which are solutions of the time-indep. S.E.:

$$\underset{\text{eigenfunction}}{\hat{H}\,\psi_n(x)} = \overset{\text{eigenvalue}}{E_n}\,\psi_n(x)$$

} eigenvalue equation for operator $\hat{H}$

- stationary: $|\psi(x)|^2$ is time independent, and so are all expectation values!

$\Rightarrow$ stationary states are orthonormal:

$$\int_{-\infty}^{+\infty} \psi_m^*(x)\,\psi_n(x)\,dx = \delta_{nm}$$

Kronecker delta

$$\delta_{nm} = \begin{cases} 1, & \text{if } m = n \\ 0, & \text{if } m \neq n \end{cases}$$

$\Rightarrow$ define inner product of two functions $\psi_n$ and $\psi_m$

$$\boxed{\langle \psi_m | \psi_n \rangle \equiv \int_{-\infty}^{+\infty} \psi_m^*(x)\,\psi_n(x)\,dx}$$

$\Rightarrow$ will give this later a much more general meaning ...

$\Rightarrow$ time-dep. S.E. is linear in $\Psi(x,t)$

$\Rightarrow$ any general solution of the time-dep. S.E. for a given potential can be written as a superposition of the stationary states:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-i\frac{E_n}{\hbar}t}$$

$\Rightarrow$ expansion of $\Psi(x,t)$ in terms of stationary states!

- $|\Psi(x,t)|^2$ is time dependent
  - $\Rightarrow$ by superposition one can built up wave packets corresponding to "moving particles"
- $c_n$'s: complex numbers

⇒ coefficient $c_n$ are given by

$$c_n = \int_{-\infty}^{+\infty} \psi_n^*(x)\, \Psi(x, t=0)\, dx$$

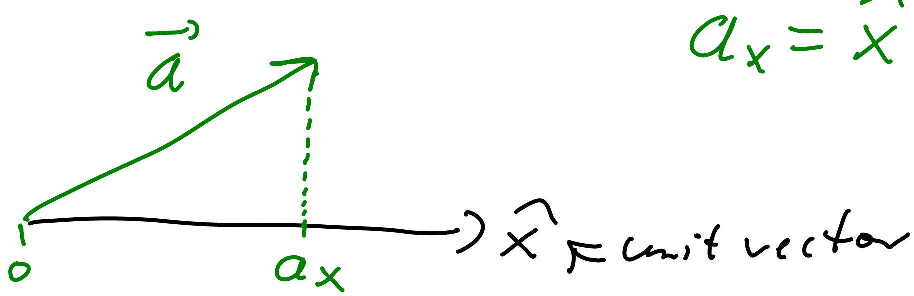
$$= \langle \psi_n | \Psi(x, t=0) \rangle$$

with the initial condition:

$$\Psi(x, t=0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

$$\Rightarrow c_n = \langle \psi_n | \Psi(t=0) \rangle$$ = "projection amplitude" of $\Psi(t=0)$ onto the state state $\psi_n$

analog to vectors:




$a_x = \hat{x} \cdot \vec{a}$ = projection amplitude of vector $\vec{a}$ onto x-axis

**A bound particle in a potential well is described by the following initial wavefunction at t = 0:**

$$\Psi(x,t=0)=\underbrace{\sqrt{\frac{3}{4}}}_{c_1}\psi_1(x)+\underbrace{\frac{1}{2}}_{c_2}\psi_2(x)$$

**Here $\psi_1(x)$ is the ground stationary state with energy $E_1$, and $\psi_2(x)$ is the second stationary state with energy $E_2$. The functions $\psi_1(x)$ and $\psi_2(x)$ are normalized. What is the probability that a measurement of energy would give $E_2$ as result?**

**A. 0**

**B. ¼**

**C. ½**

**D. 1**

**E. Something else**

$|c_2|^2 =$ prob. of measuring $E_2$

$= |\langle \psi_2 | \Psi(x,t=0)\rangle|^2$

$= \left| \sqrt{\tfrac{3}{4}} \underbrace{\langle \psi_2 | \psi_1 \rangle}_{=0 \text{ since states are orthogonal}} + \tfrac{1}{2} \underbrace{\langle \psi_2 | \psi_2 \rangle}_{=1\text{, since states are normalized}} \right|^2$

$= |\tfrac{1}{2}|^2 = 1/4$

⇒ Interpretation of coefficients $c_n$:

$|c_n|^2$ = probability, that a measurement of the energy of the particle would give the value $E_n$

Important: only possible results are $E_1, E_2, E_3 \ldots$ i.e. the eigenenergies for $\hat{H}$

- $\sum_{n=1}^{\infty} |c_n|^2 = 1$ = sum of probabilities

- Expectation value of energy:

$$\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

## III$_2$ Hilbert Space:

Quantum Theory: two constructs

→ wave functions: represent the state of the particle

→ operators: represent observables

- wave function: must be normalizable:

$$\int_{-\infty}^{+\infty} |\Psi|^2 dx = 1 \quad \langle \Psi | \Psi \rangle$$

⇒ set of all square integrable functions on a specified interval, $(a, b)$ [for us in QM: $a = -\infty$, $b = +\infty$] $f(x)$ such that $\int |f(x)|^2 dx < \infty$ is called a Hilbert space (by physicists)

⇒ $\boxed{\text{wave functions live in Hilbert space}}$

## Which of these functions is in Hilbert space for the interval 0 to +1?

A. f(x) = 1/x

B. f(x) = 1/√x

C. f(x) = x

D. All of the above

E. None of the above

need: $\int_0^1 |f(x)|^2 dx < \infty$

$\int_0^1 \frac{1}{x^2} dx = \left[-\frac{1}{x}\right]_0^1 = \infty$ No

$\int_0^1 \frac{1}{x} dx = \ln(1) - \ln(0) = \infty$ No

$\int_0^1 x^2 dx = \left[\frac{x^3}{3}\right]_0^1 < \infty$ ✓

- define inner product of two functions $f(x), g(x)$ in Hilbert space:

$$\langle f | g \rangle \equiv \int_a^b f^*(x)\, g(x)\, dx \quad \text{(always finite)}$$

Note:

$$\langle f | g \rangle = \langle g | f \rangle^*$$

$\Rightarrow$ complex conjugate of an inner product reverses the order

- inner product of a function with itself:

$$\langle f | f \rangle = \int_a^b |f(x)|^2 dx$$

$\Rightarrow$ real, non-zero $\quad [\langle f | f \rangle = \langle f | f \rangle^*]$

$\Rightarrow$ function is normalized, if $\langle f | f \rangle = 1$

- a set of functions $\{f_n\}$ in Hilbert space is orthonormal if

$$\langle f_m | f_n \rangle = \delta_{nm}$$

- a set of functions $\{f_n\}$ is complete, if any other function $f(x)$ (in Hilbert space) can be expressed as a linear combination of them:

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$$

$\Rightarrow$ if the functions $\{f_n\}$ are orthonormal, the coefficients $c_n$ are given by

$$c_n = \langle f_n | f \rangle$$

Example: complete, orthonormal set of bound stationary state wave functions!