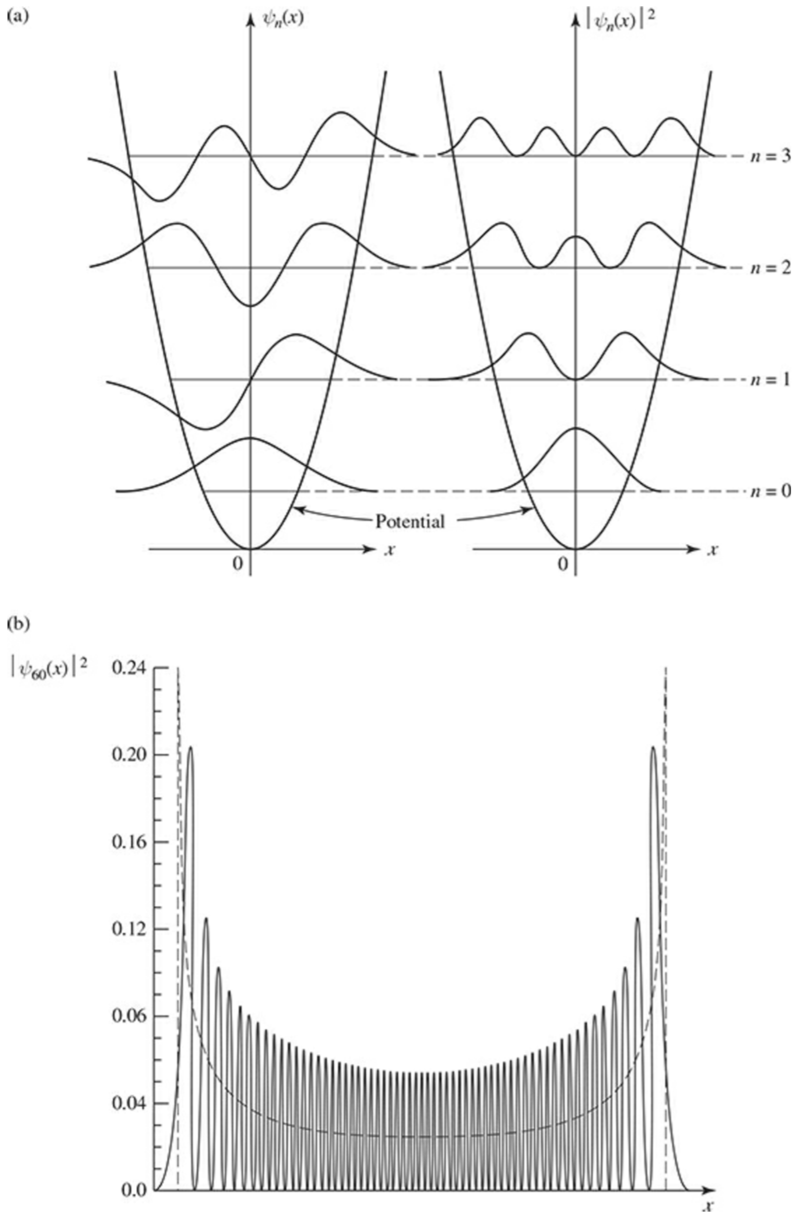
Today in Physics 237: normalization, non-normalizability

- Normalizing the wavefunctions for the quantum simple harmonic oscillator
- Outline of the analytical solution to the Schrödinger equation for the quantum simple harmonic oscillator
- The free particle: travelling-wave Schrödinger-equation solutions



Finishing touches to 1-D QSHO, operator-algebra style:

- Last time we found the ground state of the quantum simple harmonic oscillator, and the ladder operators which can generate the spectrum of this system's states:

$$\psi_0(x)=A_0e^{-m\omega x^2/\hbar} \quad , \quad \hat{a}_\pm=\frac{1}{\sqrt{2m\hbar\omega}}\left(\mp i\hat{p}+m\omega x\right) \quad .$$

- Implicit in this is the spectrum of states: $\boxed{\psi_v(x)=A_v\left(\hat{a}_+\right)^v e^{-m\omega x^2/\hbar} \text{ and } E_v=\left(v+1/2\right)\hbar\omega \quad ;}$ implicit also is the other part of the separation solution, $\varphi(t)=e^{-iE_nt/\hbar}$.

- It remains to find the normalizing factor A_v. This goes quickest with a lemma about the ladder operators:

For any square-integrable functions $f(x)$ and $g(x)$, $\int\limits_{-\infty}^{\infty} f^*\left(\hat{a}_\pm g\right)dx=\int\limits_{-\infty}^{\infty}\left(\hat{a}_\mp f\right)^* g\,dx$. Proof:

$$\int\limits_{-\infty}^{\infty} f^*\left(\hat{a}_\pm g\right)dx=\frac{1}{\sqrt{2m\hbar\omega}}\int\limits_{-\infty}^{\infty} f^*\left(\mp\hbar\frac{d}{dx}+m\omega x\right)g\,dx=\frac{1}{\sqrt{2m\hbar\omega}}\left[\int\limits_{-\infty}^{\infty} f^*\left(\mp\hbar\frac{d}{dx}\right)g\,dx+m\omega\int\limits_{-\infty}^{\infty} xf^*g\,dx\right]$$

Finishing touches (continued)

- With $u = f^*, du = \frac{df^*}{dx}dx, dv = \frac{dg}{dx}dx, v = g,$ do the first of these integrals by parts, and note that $\mp i\hbar = (\pm i\hbar)^*$:

$$\mp\hbar\int_{-\infty}^{\infty} f^*\frac{dg}{dx}gdx = uv\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} vdx = \mp\hbar\,\cancelto{0}{f^*g\Big|_{-\infty}^{\infty}} - (\mp\hbar)\int_{-\infty}^{\infty}\frac{df^*}{dx}gdx = -\int_{-\infty}^{\infty}\left(\mp\hbar\frac{df}{dx}\right)^* gdx \quad .$$

- Put this result into the last expression on the previous page:

$$\int_{-\infty}^{\infty} f^*(\hat{a}_{\pm}g)dx = \frac{1}{\sqrt{2m\hbar\omega}}\left[-\int_{-\infty}^{\infty}\left(\mp\hbar\frac{df}{dx}\right)^* gdx + m\omega\int_{-\infty}^{\infty} xf^*gdx\right] = \frac{1}{\sqrt{2m\hbar\omega}}\left[-\int_{-\infty}^{\infty}(\mp i\hat{p}f)^* gdx + m\omega\int_{-\infty}^{\infty} xf^*gdx\right]$$

$$= \frac{1}{\sqrt{2m\hbar\omega}}\left[\int_{-\infty}^{\infty}\Big(+[\pm i\hat{p}f]^* g + \big[m\omega xf^*\big]g\Big)dx\right] = \int_{-\infty}^{\infty}(\hat{a}_{\mp}f)^* gdx \quad \boxed{\text{, q.e.d.}}$$

Finishing touches (continued)

- It is also handy to note that, since $\hat{H}\psi_v = \hbar\omega\left(\hat{a}_\pm a_\mp \pm \frac{1}{2}\right)\psi_v = \hbar\omega\left(v + \frac{1}{2}\right)\psi_v$, $\boxed{\hat{a}_+\hat{a}_-\psi_v = v\psi_v \quad \text{and} \quad \hat{a}_-\hat{a}_+\psi_v = (v+1)\psi_v}$.
  - Applied to an excited state, $\hat{a}_+\hat{a}_-$ returns the same state, times the number of $\hbar\omega$s in its energy above the ground state.

- Onward to normalize $\hat{a}_\pm\psi_v$. Suppose that $\hat{a}_+\psi_v = c_v\psi_{v+1}$ and $\hat{a}_-\psi_v = d_v\psi_{v-1}$, where c_v and d_v are constants. Now,

$$\int_{-\infty}^{\infty} \left(\hat{a}_\pm\psi_v\right)^* \left(\hat{a}_\pm\psi_v\right) dx = \int_{-\infty}^{\infty} \left(\hat{a}_\mp\hat{a}_\pm\psi_v\right)^* \psi_v dx$$

according to our new lemma on pages 2-3

$$\left\{\begin{matrix} |c_v|^2 \\ |d_v|^2 \end{matrix}\right\} \int_{-\infty}^{\infty} \psi_{v\pm1}^*\psi_{v\pm1} dx = \left\{\begin{matrix} v+1 \\ v \end{matrix}\right\} \int_{-\infty}^{\infty} \psi_v^*\psi_v dx$$

by definition (LHS), and by the Handy expressions above (RHS)

$$\Rightarrow \quad |c_v|^2 = v+1 \quad , \quad |d_v|^2 = v$$

since we suppose that A_v, on page 2, is the correct normalization factor for ψ_v, etc.

Finishing touches (continued)

- Thus $\boxed{\hat{a}_+\psi_v = \sqrt{v+1}\,\psi_{v+1} \text{ and } \hat{a}_-\psi_v = \sqrt{v}\,\psi_{v-1} \quad .}$

- These expressions give us the ratios of the normalization factors A_v, so we can start at the ground state and work our way up from ψ_0:

$$\psi_1 = \frac{1}{\sqrt{1}}\hat{a}_+\psi_0 \quad , \quad \psi_2 = \frac{1}{\sqrt{2}}\hat{a}_+\psi_1 = \frac{1}{\sqrt{2\cdot 1}}\left(\hat{a}_+\right)^2\psi_0 \quad , \quad \psi_3 = \frac{1}{\sqrt{3}}\hat{a}_+\psi_2 = \frac{1}{\sqrt{3\cdot 2\cdot 1}}\left(\hat{a}_+\right)^3\psi_0 \quad ,$$

$$\psi_4 = \frac{1}{\sqrt{4}}\hat{a}_+\psi_3 = \frac{1}{\sqrt{4\cdot 3\cdot 2\cdot 1}}\left(\hat{a}_+\right)^3\psi_0 \quad \ldots \quad \boxed{\psi_v = \frac{1}{\sqrt{v!}}\left(\hat{a}_+\right)^v\psi_0} \quad ,$$

where, as we found last lecture, $\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} \quad .$

- The states of different v are orthogonal too:

Finishing touches (continued)

$$\int_{-\infty}^{\infty} \psi_u^* \left(\hat{a}_+\hat{a}_-\right)\psi_v dx = v\int_{-\infty}^{\infty} \psi_u^*\psi_v dx$$

by the Handy expressions at the top of page 4

$$\int_{-\infty}^{\infty} \left(\hat{a}_-\psi_u\right)^* \left(\hat{a}_-\psi_v\right) dx =$$

by the lemma on pages 2-3

$$\int_{-\infty}^{\infty} \left(\hat{a}_+\hat{a}_-\psi_u\right)^* \psi_v dx =$$

by the lemma again

$$u\int_{-\infty}^{\infty} \psi_u^*\psi_v dx =$$

by those Handy expressions again

- If $u \neq v$, this requires $\int_{-\infty}^{\infty} \psi_u^*\psi_v dx = 0$. And since the ψ_v are normalized, $\boxed{\int_{-\infty}^{\infty} \psi_u^*\psi_v dx = \delta_{uv}}$.
- So the ψ_v for the 1-D quantum simple harmonic oscillator are a complete orthonormal set of functions, permitting Fourier series formulation of the time-dependent wavefunctions and Fourier’s Trick, just like the infinite square well.

Now for the hard way.

We won’t do this in detail though.

- Back to the time-independent Schrödinger equation: $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi=E\psi$.
- Make some abbreviations: $\xi=\sqrt{\frac{m\omega}{\hbar}}x$, $K=\frac{2E}{\hbar\omega}$ $\Rightarrow$ $\left(\frac{d^2}{d\xi^2}-\xi^2+K\right)\psi=0$. This looks hard to solve, and is.
- To make a long and complicated story short: this equation has the solution

$$\psi_v(\xi)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^v v!}}H_v(\xi)e^{-\xi^2/2} \quad , \quad \text{with eigenvalues } K_v=2v+1 \quad , \quad v=1,2,...$$

  and where the functions $H_v(\xi)$ are the **Hermite polynomials**.

- Note that, as expected from the solution we got via operator algebra, it contains a Gaussian factor, and familiar normalization factors.

The hard way (continued)

- Compare apples to apples:

$$\psi_v(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{v!}}\frac{1}{\sqrt{2^v}}H_v\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-m\omega x^2/2\hbar} \quad , \quad E_v=\hbar\omega\left(v+\frac{1}{2}\right) \quad , \quad v=0,1,2,...$$

$$\psi_v(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{v!}}(\hat{a}_+)^v e^{-m\omega x^2/2\hbar} \quad , \quad E_v=\left(v+\frac{1}{2}\right)\hbar\omega \quad , \quad v=0,1,2,...$$

- The extra factor of $1/\sqrt{2^v}$ is a convention in the definition of the Hermite polynomials.

- So if you need a large-*v* wavefunction and don't have time to calculate $(\hat{a}_+)^v e^{-m\omega x^2/2\hbar}$, you can look up the Hermite polynomials in tables instead.

The hard way (continued)

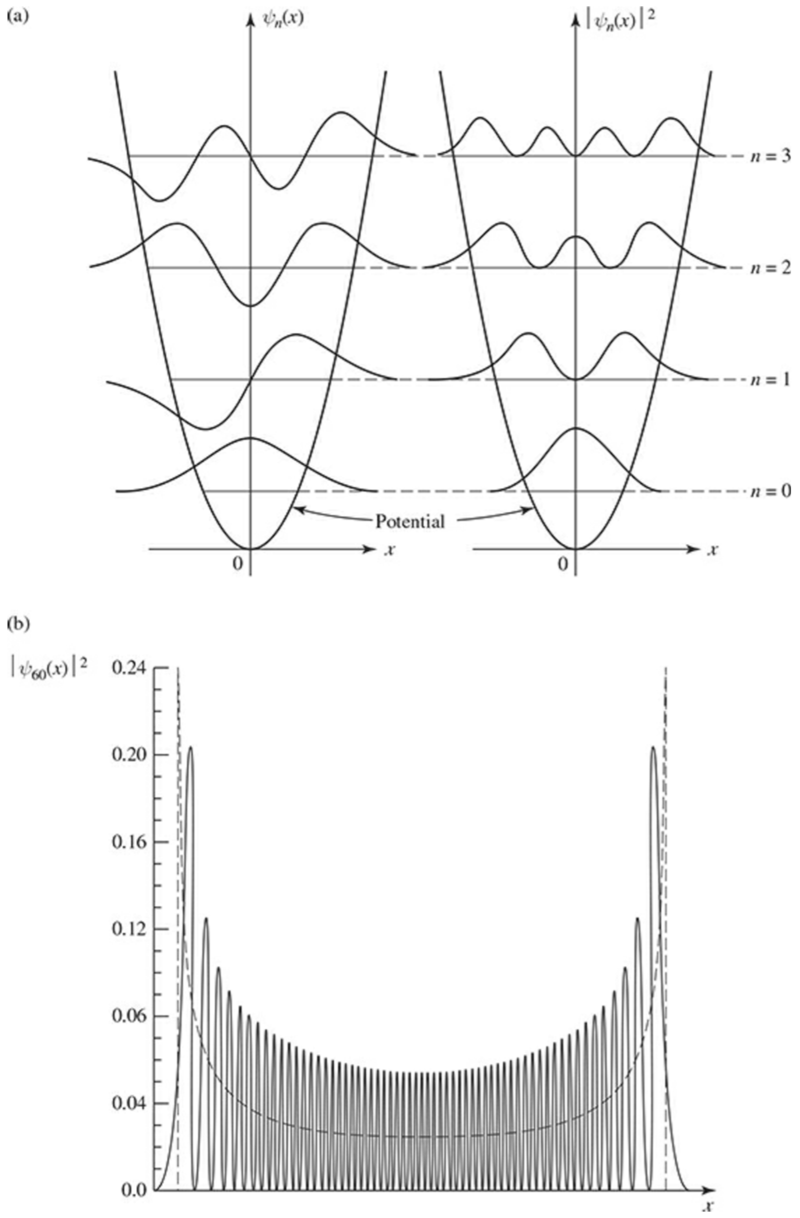
- For those experienced in MATH 281 and/or PHYS 217: the Hermite polynomials have some of the properties familiar from **Legendre polynomials**, including
    - they're just polynomials: easy to integrate.
    - they're orthonormal and complete: easy to integrate products of them, and represent functions in Fourier-like series with coefficients solvable *via* Fourier's Trick.
    - they can be computed *via* a **Rodrigues formula**, $H_v(\xi) = (-1)^v e^{\xi^2} \left(\frac{d}{d\xi} \right)^v e^{-\xi^2}$, which looks a lot like the product-of-creation-operators version (see G&S Problem 2.16a).
    - they have a generating function, $e^{-z^2 + 2z\xi}$, which preserves the form of the ground state but yields to a simple power-series expression (see G&S problem 2.16d).
        - The generating function of Legendre polynomials is $1/\mathscr{r} = 1/|\boldsymbol{r} - \boldsymbol{r}'|$, for which the power-series representation leads to the definition and use of multipole moments in electrostatics and magnetostatics.
        - … and is why we will see them when we deal with the hydrogen atom.

The hard way (continued)

- The first six Hermite polynomials:

$$
\begin{aligned}
H_0 &= 1, \\
H_1 &= 2\xi, \\
H_2 &= 4\xi^2 - 2, \\
H_3 &= 8\xi^3 - 12\xi, \\
H_4 &= 16\xi^4 - 48\xi^2 + 12, \\
H_5 &= 32\xi^5 - 160\xi^3 + 120\xi.
\end{aligned}
$$

Note that they alternate between even and odd with respect to their argument, as Legendre polynomials also do.



The free quantum

- The simplest looking case, but a subtle one.
- The time-independent Schrödinger equation for the free quantum is merely $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi = -k^2\psi$,

  same as inside the infinite square well, but this time with no boundary conditions.
- In the infinite square well, the boundary conditions "chose" standing waves, for which sine and cosine particular solutions are most convenient.
- Perforce, the free quantum travels, and we will find the Euler-formula equivalent, complex exponential solutions handier:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

$$\Psi(x,t) = Ae^{ikx-iEt/\hbar} + Be^{-ikx-iEt/\hbar}$$

$$= Ae^{ik(x-\hbar kt/2m)} + Be^{-ik(x+\hbar kt/2m)} \quad .$$

The free quantum (continued)

- The two terms represent travelling waves, in which a peak or a wavepacket travels to +*x* (first term) or –*x* (second).
- We can bundle the two terms together by letting *k* be a signed variable:

$$k = \pm\sqrt{2mE}\big/\hbar : \quad + \text{ travels to } +x, \; - \text{ to } -x;$$

$$\Psi_k(x,t) = A_k e^{i\left(kx - \hbar k^2 t/2m\right)} \quad .$$

- Features detectable at a glance:
  - Wavelength, momentum, and speed: $\lambda = 2\pi/k$, $p = \hbar k$, $v = \hbar k/2m$.
  - Quantum speed not the same as classical: $v = \hbar k/2m = \sqrt{E/2m}$, not $E = mv^2/2 \Rightarrow v_{\text{classical}} = \sqrt{2E/m} = 2v_{\text{quantum}}$.
  - **Wavefunction not normalizable**: $\int_{-\infty}^{\infty} \left|\Psi_k(x,t)\right|^2 dx = |A|^2 \int_{-\infty}^{\infty} dx \to \pm\infty$.