Lecture 14 - Quantum Mechanics

A. The Schrödinger Equation

So, with the idea that matter is a dual wave/particle, the founders of quantum mechanics wanted to re-write mechanics in terms of wave equations

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \frac{\partial^2 \psi}{\partial x^2}. \quad \leftarrow \text{wave equation}$$

We saw above, that the wave equation has a solution for a traveling wave (in 1D)

$$\psi(x,t) = a \exp[i(kx - \omega t)]$$

We will now substitute the Planck-Einstein equations into this expression

$$\left.\begin{array}{l} E = \hbar \omega \\ \underline{p} = \hbar \underline{k} \;\longrightarrow\; \text{1D version} \quad p = \hbar k \end{array}\right\} \quad \begin{array}{l} \omega = E/\hbar \\ k = p/\hbar \end{array}$$

$$\psi(x,t) = a \exp\left(i \frac{px - Et}{\hbar}\right) \qquad (*)$$

This is a traveling "wave-particle" in free space! The founders arrived at this by intuition, by combining ideas of waves and particle mechanics. We would like to go backwards and find a differential equation that is consistent with this solution. Then, perhaps, we can solve more complex problems. What follows here is not really a derivation. It is more like the reasoning the founders of QM used to arrive at the Schrödinger Equation.

Let's first look at the time-dependence. To do this we will take the time derivative of $(*)$. Taking the time derivative gives,

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar}\, a \exp\left(i\,\frac{px - Et}{\hbar}\right)$$

$$(i\hbar)\,\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar}\,\psi\,(i\hbar) \Rightarrow \quad i\hbar\frac{\partial \psi}{\partial t} = E\psi$$

We will pause there for now, and look at the spatial dependence next. Taking the derivative of (✱) with respect to space twice,

$$\frac{\partial \psi}{\partial x} = \frac{ip}{\hbar}\, a \exp\left(i\,\frac{px - Et}{\hbar}\right) = \frac{ip}{\hbar}\,\psi$$

$$\frac{\partial^2 \psi}{\partial x^2} = \left(\frac{ip}{\hbar}\right)^2 \psi = -\frac{p^2}{\hbar^2}\,\psi \Rightarrow -\hbar^2\frac{\partial^2 \psi}{\partial x^2} = p^2\psi \, .$$

Recall that the energy of a freely moving particle consists of the kinetic energy only

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} \quad \Rightarrow p^2 = 2mE \Rightarrow \frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = E\psi$$

Putting both the time derivative and the spatial derivative together,

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \quad \Rightarrow \quad i\hbar\frac{\partial \psi}{\partial t} = \hat{H}\psi$$

Hamiltonian

For a particle in a potential, the Hamiltonian is actually

$$\hat{H} = \hat{K} + \hat{U} = \frac{p^2}{2m} + \hat{U}\, ,$$

and the differential equation can be written as

$$i\hbar\frac{\partial \psi}{\partial t} = \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right]\psi$$

What did we do?

- We used the Planck-Einstein equations and the solution for a plane wave to provide a differential equation in terms of the particle Hamiltonian.

- Not a classical wave equation (oscillation only). Not a diffusion equation (damping only). Somewhere in between.
- More rigorously, this equation is a postulate or a law, like Newton's 2nd law.

Of course, this equation is called Schrödinger's equation. Let's write out the general, 3D Time-dependent Schrödinger Equation

$$\boxed{i\hbar \frac{\partial}{\partial t}\psi(\underline{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\underline{r},t)\right]\psi(\underline{r},t)}$$

$|\psi\rangle$ ket vector in a Hilbert space

$$\boxed{i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle}$$

$\hat{H}$: Hamiltonian operator

B. Time-Independent Schrödinger Equation

When the Hamiltonian doesn't depend on time, the time-dependent equation can be "formally" integrated,

$$|\psi(t)\rangle = \exp\left(\frac{-i}{\hbar}\hat{H}t\right)|\psi(\underline{r},0)\rangle$$

operator/matrix in an exponential

Using a spectral decomposition, this can be written as

$$\psi(\underline{r},t) = \sum_{n=0}^{\infty} c_n \exp\left(\frac{-iE_nt}{\hbar}\right)\phi_n(\underline{r})$$

More on the time-dependent solution later when we do some examples. Substituting just one of these modes (any n) into the Schrödinger Equation gives,

$$i\hbar\frac{\partial}{\partial t}\left[e^{-iE_nt/\hbar}\psi_n(r)\right] = \left[-\frac{\hbar^2}{2m}\nabla^2 + U\right]\left(e^{-iE_nt/\hbar}\psi_n(\underline{r})\right)$$

$$\cancel{i\hbar}\,\psi_n(r)\cdot\frac{-\cancel{i}E_n}{\cancel{\hbar}}\cancel{e^{-iE_nt/\hbar}} = \left[-\frac{\hbar^2}{2m}\nabla^2 + U\right]\psi(r)\,\cancel{e^{-iE_nt/\hbar}}$$

doesn't depend on x

$$E_n \psi_n(r) = \left[\frac{-\hbar^2}{2m}\nabla^2 + u\right]\psi_n(r)$$

This gives us the so-called Time-Independent Schrödinger Equation

$$\boxed{\left[\frac{-\hbar^2}{2m}\nabla^2 + u\right]\psi_n(r) = E_n\psi(r)} \qquad \boxed{\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle}$$

This is an eigenvalue problem. $|\psi_n\rangle$ is the eigenket vector or eigen-function. E_n, the energy, is the eigenvalue.

The Fourier transform of the Schrödinger equation gives an equation explicit in the momentum

$$i\hbar\frac{\partial\hat{\psi}}{\partial t} = \frac{p^2}{2m}\hat{\psi} + \frac{1}{(2\pi\hbar)^{3/2}}\underbrace{\int_{-\infty}^{\infty}\hat{u}(p-p')\,\hat{\psi}(p)\,dp'}_{\hat{u} * \hat{\psi}\,,\ F[u] = \hat{u}}$$

The Fourier transform definition

$$F[\psi] = \hat{\psi}(\underline{p}) = \frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} e^{\frac{-i\underline{p}\cdot\underline{r}}{\hbar}}\,\psi(\underline{r})\,d\underline{r}$$

$$F^{-1}[\hat{\psi}] = \psi(\underline{r}) = \frac{1}{(2\pi\hbar)^{3/2}}\int_{-\infty}^{\infty} e^{\frac{i\underline{p}\cdot\underline{r}}{\hbar}}\,\hat{\psi}(\underline{p})\,d\underline{p}$$

Note the different F.T. convention.

The F.T. conventions in these notes are inconsistent!

Note that the momentum is the Fourier conjugate variable to position.

- Uncertainty principle!
- Another reason why position and momentum are the canonical variables in the Hamiltonian.

C. Postulates of Quantum Mechanics

What is a succinct summary of the minimum set of rules we need to describe quantum mechanics? This will help us understand what quantum mechanics really is, what it means, and how to mathematically compute what we need.

(i). Classical Mechanics

1. The state of the system at time t_0 is described by specifying $3N$ generalized coordinates $q_i(t_0)$ and their conjugate momenta $p_i(t_0)$.

2. The value of any function of the q_i and p_i, $f(q_i, p_i, t)$, is determined for any time t when the initial state is specified at t_0.

3. The time evolution of the state of the system is given by Hamilton's equations,

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} \qquad H = \frac{p_i^2}{2m} + U(q_i, t)$$

(ii.) Quantum Mechanics

1. The state of the system is defined by specifying a ket vector $|\psi(t_0)\rangle$ at time t_0.

   This is equivalent to specifying a wave function $\psi(x, t_0)$ or $\hat{\psi}(p, t_0)$.

2. Every measurable physical quantity A is described by an operator $\hat{A}$ in the Hilbert space. This operator is an "observable".

   Example: The Hamiltonian operator

$$\hat{H} = \underbrace{-\frac{\hbar}{2m}\nabla^2}_{\text{Kinetic Energy operator}} + \underbrace{\hat{U}(r,t)}_{\text{Potential Energy operator}}$$

Example: Position and Momentum

$\hat{R} = \underline{r} \qquad \hat{\underline{p}} = i\hbar \underline{\nabla}$

3. The only possible measurement of a physical quantity A is one of the eigenvalues of the observable $\hat{A}$.

$$\hat{A}|\psi\rangle = A|\psi\rangle$$

Example: Energy

$\hat{H}|\psi\rangle = E|\psi\rangle$ Energy is the eigenvalue.

4. The probability of measuring an eigenvalue a_n corresponding to the physical quantity A from a system in state $|\psi\rangle$ is given by

$$P(a_n) = |\langle u_n|\psi\rangle|^2 = \left|\int_{-\infty}^{\infty} u_n(x,t)\,\psi_n(x,t)\,dx\right|^2$$

where $|u_n\rangle$ are eigenvectors corresponding to the eigenvalues a_n,

operator. this is usually a D.E.

$$\hat{A}|u_n\rangle = a_n|u_n\rangle \Rightarrow \hat{A}u_n(x,t) = a_n u_n(x,t).$$

[Aside] There is an easier way to get $P(a_n)$ using the spectral (eigenvalue) decomposition.

$|\psi\rangle = \sum_n c_n |u_n\rangle$ (spectral decomposition)

Using this expression gives

$$P(a_n) = |\langle u_n|\psi\rangle|^2 = |\langle u_n|c_n|u_n\rangle| = |c_n|^2$$

We get the c_n by using the orthonormality of the eigen-kets

$$\langle u_m|\psi\rangle = \sum_n \langle u_m|c_n|u_n\rangle$$

$$= \sum_n c_n \underbrace{\langle u_m | u_n \rangle} = c_m \qquad \delta_{mn} = \begin{cases} 1 & \text{if } m=n \\ 0 & \text{if } m \neq n \end{cases}$$

$$c_m = \langle u_m | \psi \rangle = \int_{-\infty}^{\infty} u_m(x)\,\psi(x,t)\,dx$$

5. If the measurement of the quantity A gives the value a_n, then the system immediately after becomes the eigen-ket associated with that value, $|u_n\rangle$.

$$|\psi\rangle \overset{a_n}{\Longrightarrow} \frac{c_n}{|c_n|} |u_n\rangle$$

It renormalizes. c_n could be complex, so there could be a phase shift.

6. The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t)\,|\psi(t)\rangle$$

where $H(t)$ is the observable associated with the total energy.

Some Comments:

- Postulates 3, 4, and 5 are kind of weird. Why does the wave-function "collapse" to an eigenfunction? This is what different interpretations of QM try to explain. The rest is sort of straightforward from the math.

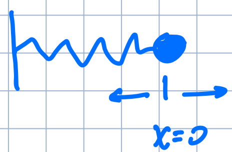
- The uncertainty principle is a consequence of the postulates, not a postulate itself. It is a natural result of the wave mechanics.

D. Numerical Solution of the quantum harmonic oscillator

- Go over numerical solution
- Talk about in context with the postulates

E. Appendix: Quantum Harmonic Oscillator

Reminder: classical Harmonic oscillator



Spring potential : $U = \frac{1}{2} k x^2 = \frac{1}{2} \omega^2 m x^2$

particle mass : m

initial conditions: $x(0) = x_0$, $v(0) = v_0$

$$m \frac{d^2x}{dt^2} = -\frac{\partial U}{\partial x}$$

$$\frac{d^2x}{dt^2} + \frac{k}{m} x = 0 \Rightarrow \frac{d^2x}{dt^2} + \omega^2 x = 0 \qquad \omega^2 = k/m \, , \; k = \omega^2 m$$

$$\boxed{\begin{aligned} x(t) &= \frac{v_0}{\omega} \sin(\omega t) + x_0 \cos(\omega t) \\ v(t) &= v_0 \cos(\omega t) - x_0 \omega \sin(\omega t) \end{aligned}}$$

Back to the Quantum Harmonic Oscillator (QHO) ...

The 1D time-dependent Schrödinger Equation is

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U \right] \psi \qquad U = \frac{1}{2} m \omega^2 x^2$$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi$$

Initial condition : $\psi(x, 0) = \psi_0(x)$

Boundary Conditions : $\psi(-\infty, t) = \psi(+\infty, t) = 0$

(i) Dimensional Analysis

First, to simplify, lets make the problem dimensionless

$$\tilde{x} = x/l \qquad \tilde{t} = t/\tau \qquad \tilde{\psi} = \frac{\psi}{l^{1/2}} \qquad \left[\psi \sim L^{-1/2} \text{ because } \int |\psi^2| dx = 1 \right]$$

Parameters? $m, \hbar, \omega$ $\quad\quad$ $m \to kg$ $\quad$ $\hbar \to J\cdot s$ $\quad$ $\omega \to 1/s$

τ is pretty straightforward. Let $\tau = 1/\omega$

ℓ is not as obvious. We can leave it and solve for it while we non-dimensionalize.

$$i\hbar\omega\,\ell^{1/2}\frac{\partial\tilde\psi}{\partial\tilde t} = -\frac{\hbar^2}{2m}\cdot\frac{\ell^{1/2}}{\ell^2}\frac{\partial^2\tilde\psi}{\partial\tilde x^2} + \frac{1}{2}m\omega^2\ell^{5/2}\tilde x^2\tilde\psi$$

- all $\ell^{1/2}$ cancel
- also divide by $\hbar\omega$

$$i\frac{\partial\tilde\psi}{\partial\tilde t} = -\frac{\hbar}{2m\omega}\frac{1}{\ell^2}\frac{\partial^2\tilde\psi}{\partial\tilde x^2} + \frac{1}{2}\frac{m\omega}{\hbar}\ell^2\tilde x^2\tilde\psi$$

$$\text{let } \frac{\hbar}{m\omega\ell^2} = 1 \Rightarrow \ell^2 = \frac{\hbar}{m\omega} \Rightarrow \ell = \left(\frac{\hbar}{m\omega}\right)^{1/2}$$

$$(*)\quad \boxed{i\frac{\partial\tilde\psi}{\partial\tilde t} = -\frac{1}{2}\frac{\partial^2\tilde\psi}{\partial\tilde x^2} + \frac{1}{2}\tilde x^2\tilde\psi} \quad \boxed{\tilde x = x\left(\frac{m\omega}{\hbar}\right)^{1/2},\quad \tilde t = \omega t}$$

The dimensionless equation has the natural length $\left(\ell = \sqrt{\hbar/m\omega}\right)$ and time $(\tau = 1/\omega)$ units for this problem.

Quick units check: $\quad \dfrac{\hbar}{m\omega} = \dfrac{J\cdot s}{kg\; 1/s} = \dfrac{kg\, m^2/s^2 \cdot s}{kg/s} = m^2$ ✓

$$\frac{1}{\omega} = \frac{1}{1/s} = s \checkmark$$

Now we can focus on the math and add the units / parameters back later when we want them.

(ii) Separation of variables

The equation $(*)$ is a linear PDE. It is 1^{st} order in time and second order in space. It is complex. There are various methods of solution. We will use the method of separation of variables.

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}x^2\psi$$

- Drop the tildes.
- Sort of like a diffusion equation with a spatially dependent reaction (but complex time).

Assume the form of a product solution:

$$\psi = f(t)g(x)$$

$$i\frac{\partial(fg)}{\partial t} = -\frac{1}{2}\frac{\partial^2(fg)}{\partial x^2} + \frac{1}{2}x^2 fg$$

$$ig\frac{\partial f}{\partial t} = -\frac{1}{2}f\frac{\partial^2 g}{\partial x^2} + \frac{1}{2}x^2 fg$$ Divide by fg

$$\underbrace{\frac{i}{f}\frac{\partial f}{\partial t}}_{\text{only depends on } t} = \underbrace{-\frac{1}{2}\frac{1}{g}\frac{\partial^2 g}{\partial x^2} + \frac{1}{2}x^2}_{\text{only depends on } x} = \lambda$$ Must equal a constant.

We've divided our PDE into two ODEs. One is an ODE-IVP in time. The other is an ODE-BVP in space

① $$\frac{i}{f}\frac{df}{dt} = \lambda \Rightarrow \frac{df}{dt} = -i\lambda f$$

② $$-\frac{1}{2}\frac{1}{g}\frac{d^2 g}{dx^2} + \frac{1}{2}x^2 = \lambda \Rightarrow -\frac{1}{2}\frac{d^2 g}{dx^2} + \frac{1}{2}x^2 g = \lambda g$$

This is an eigenvalue problem

$$\mathcal{L}g = \lambda g \quad , \quad \mathcal{L} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2}$$

eigenvalue

differential operator
Has eigenfunction solutions.

(iii) Solve ODE #1

$$\frac{df}{dt} = -i\lambda f \Rightarrow \frac{1}{f}df = -i\lambda\, dt \Rightarrow \ln f = -i\lambda t + \text{const}$$

$$\boxed{f(t) = \text{const} \exp(-i\lambda t)}$$

(iv) Solve ODE #2 (time independent Schrödinger equation)

$$-\frac{1}{2}\frac{d^2 g}{dx^2} + \frac{1}{2}x^2 g = \lambda g \Rightarrow \frac{d^2 g}{dx^2} - x^2 g = -2\lambda g$$

$$\frac{d^2 g}{dx^2} + (2\lambda - x^2) g = 0$$

This is a 2nd order, non-constant coefficient ODE. Non-constant coefficient ODEs are special cases. (Remember Bessel functions, spherical Bessel functions, etc.)

It turns out this ODE is more well-known in a different form. We need to change variables to be able to look it up and use numerical packages.

Let $g(x) = \exp(-x^2/2)\, h(x)$

[Aside] Work out the transformation:

$$\frac{dg}{dx} = -x e^{-x^2/2} h(x) + e^{-x^2/2} \frac{dh}{dx}$$

$$\frac{d^2 g}{dx^2} = -e^{-x^2/2} h(x) + x^2 e^{-x^2/2} h(x) - x e^{-x^2/2} \frac{dh}{dx} - x e^{-x^2/2} \frac{dh}{dx} + e^{-x^2/2} \frac{d^2 h}{dx^2}$$

$$= (x^2 - 1) e^{-x^2/2} h - 2x e^{-x^2/2} \frac{dh}{dx} + e^{-x^2/2} \frac{d^2 h}{dx^2}$$

Substitute into the original ODE:

$$\left[(x^2-1)h - 2x\frac{dh}{dx} + \frac{d^2 h}{dx^2}\right] \cancel{e^{-x^2/2}} + (2\lambda - x^2)\cancel{e^{-x^2/2}} h = 0$$

$$\frac{d^2h}{dx^2} - 2x\frac{dh}{dx} + (x^2 - 1 + 2\lambda - x^2)h = 0$$

$$\boxed{\frac{d^2h}{dx^2} - 2x\frac{dh}{dx} + (2\lambda - 1)h = 0}$$

This equation is called Hermite's differential equation.

This is a singular Sturm-Liouville eigenvalue problem.

$$\mathcal{L}h = \gamma h, \quad \mathcal{L} = \frac{d^2}{dx^2} - 2x\frac{d}{dx}, \quad \gamma = 2\lambda - 1$$

Solutions to Hermites DE are given by a sum of linearly independent eigenfunctions

$$h(x) = c_1 H_n(x) + c_2 Y_n(x) \quad \text{where} \quad \gamma = 2n \quad n = 0, 1, 2, ..$$

Hermite polynomials (of the 1^{st} kind)

Hermite functions of the 2^{nd} kind

eigenvalues

$$2\lambda - 1 = 2n$$
$$\lambda = n + 1/2$$

[Aside] How do we calculate $H_n(x)$ and $Y_n(x)$?

The $H_n(x)$ can be obtained by the expression

$$H_n(x) = (-1)^n e^{x/2} \frac{d^n}{dx^n}\left(e^{-x^2}\right)$$

$$H_0(x) = 1$$

$$H_1(x) = (-1)\, e^{x^2} \frac{d}{dx}\left(e^{-x^2}\right) = -e^{x^2}\left(-2x e^{-x^2}\right) = 2x$$

$$H_2(x) = (-1)^2 e^{x^2} \frac{d^2}{dx^2}\left(e^{-x^2}\right) = e^{x^2}\left(-2e^{-x^2} + 4x^2 e^{-x^2}\right)$$
$$= 4x^2 - 2$$

$$H_3(x) = 8x^3 - 12x, \quad H_4(x) = 16x^4 - 48x^2 + 12$$

from wikipedia

Let's check to make sure these are actually solutions.

$$\frac{d^2 H_n}{dx^2} - 2x\frac{dH_n}{dx} + 2n H_n(x) = 0$$

$n=0$: $H_0 = 1 \quad \frac{dH_0}{dx} = 0 \quad \Rightarrow \quad 0 - 2x\cdot 0 + 2\cdot 0\cdot 1 \stackrel{?}{=} 0$ ✓

$n=1$: $H_1 = 2x \quad \frac{dH_1}{dx} = 2 \quad \frac{d^2H_1}{dx^2} = 0 \quad \Rightarrow \quad 0 - 2x\cdot 2 + 2\cdot 1\cdot 2x \stackrel{?}{=} 0$ ✓

$n=2$: $H_2 = 4x^2 - 2 \quad \frac{dH_2}{dx} = 8x \quad \frac{d^2H_2}{dx^2} = 8 \Rightarrow \quad 8 - 2x(8x) + 2\cdot 2\cdot(4x^2-2) \stackrel{?}{=} 0$ ✓

The problem is finding what is tabulated. Kummer's DE is given by

$$z\frac{d^2w}{dz^2} + (b-z)\frac{dw}{dz} - aw = 0$$

It has solutions $M(a,b,z)$ and $U(a,b,z)$ which are called confluent hypergeometric functions of the first (M) and second (U) kind.

These also come up in the Graetz problem in forced convection.

Alternate notation for M is:

$M(a,b,z) = {}_1F_1(a,b,z)$ ← notation for generalized hypergeometric series

"hyp1f1" is the name of the Python function

One can write Hermite polynomials and functions using confluent hypergeometric functions.

$H_n(x) = 2^n U(-\frac{n}{2}, \frac{1}{2}, x^2)$ ← hyperu is the Python function.

$Y_n(x) = M(-\frac{n}{2}, \frac{1}{2}, x^2)$

M is also known as Kummer's confluent hypergeometric function.

U is also known as Tricomi's confluent hypergeometric function.

The $Y_n(x)$ cannot be physical solutions. They diverge to infinity at points in the domain, so $|\psi|^2 \not< \infty$. So, these cannot be wave functions. ($Y_n(x)$ are not compatible with B.C.'s).

we now have the solution for $g(x)$

$$g(x) = c \cdot e^{-x^2/2} \cdot H_n(x)$$

[Aside] The $g(x)$ need to be normalized so that

$$\langle g_n(x) | g_n(x) \rangle = \int_{-\infty}^{\infty} g_n(x)\, g_n^*(x)\, dx = 1$$

← complex conjugate

use this to solve for c

This will give us a proper probability density. I found these values and verified using Mathematica.

$$c_n = \left(2^n n! \sqrt{\pi}\right)^{-1/2}$$

The integrals for Ψ_n only converge for $n \in$ even. This is why they are not physical. But for the even ones, the normalization constant is

$$c_n = \left(2^n \underbrace{\frac{(n/2)!^2}{n!}}\sqrt{\pi}\right)^{-1/2}$$

Wow! chatGPT recognized this sequence as the central binomial coefficients. Super cool!

After normalizing, we have our complete set of orthonormal basis functions, and the solution to the problem in the x-direction.

$$g_n(x) = c_n e^{-x^2/2} H_n(x) \qquad c_n = \left(2^n n! \sqrt{\pi}\right)^{-1/2}$$

$$\lambda_n = n + 1/2, \quad n = 0, 1, \ldots, \infty$$

where the orthonormal property of $g_n(x)$ says that

$$\langle g_n | g_m \rangle = \delta_{nm} = \begin{cases} 0, & n \neq m \\ 1, & n = m \end{cases}$$

$$\int_{-\infty}^{\infty} g_n(x)\, g_m(x)\, dx = \delta_{nm}$$

(v) Product solution

Now we can put our two solutions together,

$$\psi(x,t) = f(t)\,g(x) = A_n \exp(-i\lambda_n t)\, c_n \exp(-x^2/2)\, H_n(x).$$

$\leftarrow$ coefficient for I.C.

By superposition, a sum of solutions is also a solution, so the general solution is

$$\boxed{\psi(x,t) = \sum_{n=0}^{\infty} A_n c_n \exp(-i\lambda_n t - x^2/2)\, H_n(x) \qquad \lambda_n = n + 1/2 \qquad c_n = (2^n n! \sqrt{\pi})^{-1/2}}$$

(vi) Initial condition

The last thing we need to do is use the initial condition to determine the A_n.

Let the initial state be $\psi_0(x)$. For example, it could be

$$\psi_0(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(x-x_0)^2}{2\sigma^2}\right)$$

A Gaussian wave packet.

The coefficients are given by

$$A_n = \langle \psi_0 | g_n \rangle$$

$$A_n = \int_{-\infty}^{\infty} \psi_0(x)\, g_n(x)\, dx = \int_{-\infty}^{\infty} \psi_0(x)\, c_n e^{-x^2/2} H_n(x)\, dx$$

We need to evaluate this integral for each n. We can do this numerically. Hopefully $A_n \to 0$ as $n \to \infty$ quickly, so our infinite sum converges and we don't have to do too many integrals.

[Aside] Proof of formula for A_n

$$\langle \psi_0 | g_n \rangle = \int_{-\infty}^{\infty} \psi_0(x)\, g_n(x)\, dx = \int_{-\infty}^{\infty} \underbrace{\left[\sum_{m=0}^{\infty} A_m \exp(0) \cdot g_m(x) \right]}_{\text{spectral representation of } \psi_0(x)} g_n(x)\, dx$$

$$= \sum_{m=0}^{\infty} A_m \int_{-\infty}^{\infty} g_n(x)\, g_m(x)\, dx = \sum_{m=0}^{\infty} A_m \delta_{mn} = A_n \quad \checkmark$$

(vii) Closing comments

- The eigenvalue λ_n is the dimensionless energy.

$$\lambda_n = \frac{E_n}{\hbar\omega}, \qquad E_n = \hbar\omega\,(n + 1/2), \quad n = 0, 1, 2, \ldots$$

units: $\hbar\omega = J \cdot s \cdot \frac{1}{s}$ ✓

We can see this because the eigenvalue problem for $g(x)$ is the time-independent Schrödinger equation.

- In the classical problem, the energy is continuous. Any value is allowed. In the quantum problem this is not so.

- One may also want to look at the momentum. What is the dimensionless momentum?

$$p = \hbar k = \frac{\hbar}{\ell}\tilde{k} \qquad \tilde{k} = \ell k \qquad \ell = \sqrt{\frac{\hbar}{m\omega}}$$

$$\tilde{p} = \frac{p\ell}{\hbar} = \tilde{k} \Rightarrow p = \tilde{p}\,\frac{\hbar}{\ell} = \hbar\sqrt{\frac{m\omega}{\hbar}}\,\tilde{k} = \sqrt{m\omega\hbar}\,\tilde{k}$$

$$\tilde{p} = \tilde{k} = \frac{p}{(\hbar m\omega)^{1/2}}$$

check units:

$$\hbar m\omega = J \cdot s \cdot kg \cdot 1/s = \frac{kg\, m^2}{s^2} \cdot kg = kg^2 m^2/s^2$$

$$(\hbar m\omega)^{1/2} = kg\, m/s \quad \checkmark \quad \text{(momentum)}$$