(16) Life in 3D

1 Last Time

- Our first encounter with non-Hermitian operators (QHO)
- Our last adventure in 1D

2 This Time

- Generalization to 3D
- Selected 3D examples

3 Generalization to 3D

Thus far we have been working in 1D, but the real world has 3 spatial dimensions. How do we generalize the Schrödinger equation to 3D?

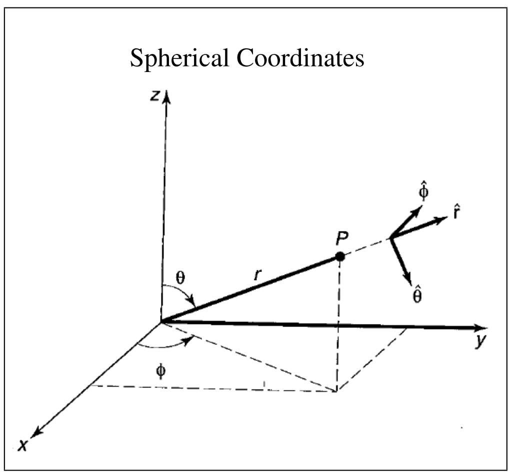
Schrödinger equation in 3D

$$
\begin{aligned}
i\hbar\partial_t &= \hat{E} \quad \text{e.g., same as 1D} \\
\hat{E} &= \frac{\hat{p}^2}{2m} + V(\vec{r}) \\
\text{but} \quad \hat{p} &= -i\hbar\vec{\nabla} = -i\hbar(\hat{e}_x\,\partial_x + \hat{e}_y\,\partial_y + \hat{e}_z\,\partial_z) \\
\Rightarrow \; i\hbar\,\partial_t\psi(\vec{r},t) &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r},t) \\
&= \left[-\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_x^2) + V(\vec{r})\right]\psi(\vec{r},t)
\end{aligned}
$$

If we were to work in spherical coordinates, on the other hand, we would have

Laplacian in Spherical Coordinates (r, θ, ϕ)

$$\begin{aligned}
x &= r \sin\theta\ \cos\phi \\
y &= r \sin\theta\ \sin\phi \\
z &= r \cos\theta \\
\nabla^2 &= \partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\left(\partial_\theta^2 + \cot\theta\,\partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2\right) \\
&= \frac{1}{r}\partial_r^2\, r + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta\right) + \frac{1}{\sin^2\theta}\partial_\phi^2\right] \\
&= \frac{1}{r^2}\left[\partial_r\left(r^2\,\partial_r\right) + \frac{1}{\sin\theta}\partial_\theta\left(\sin\theta\,\partial_\theta\right) + \frac{1}{\sin^2\theta}\partial_\phi^2\right]
\end{aligned}$$



Or, depending on the potential, we could use cylindrical coordinates.

Laplacian in Cylindrical Coordinates (ρ, ϕ, z)

$$\begin{aligned}
x &= \rho\cos\phi \\
y &= \rho\sin\phi \\
\nabla^2 &= \partial_\rho^2 + \frac{1}{\rho}\partial_\rho + \frac{1}{\rho^2}\partial_\phi^2 + \partial_z^2
\end{aligned}$$

So, the generalization is conceptually simple, though it can be mathematically complicated. Let's see how some of our favorite 1D potentials look in 3D.

4 Example: Free Particle

The simplest potential is, well, zero. That is, the potential of a free particle with no forces acting on it. In this case our energy eigenstates take on a form very similar to the 1D plane wave.

Free Particle in 3D

$$
\begin{aligned}
V(\vec{r}) &= 0 \qquad \text{no forces} \\
\Rightarrow \hat{E} &= \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_x^2)
\end{aligned}
$$

To find energy eigenstates we should solve

EES of Free Particle in 3D

$$
\begin{aligned}
i\hbar\,\partial_t\psi(\vec{r}) &= -\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_x^2)\psi(\vec{r}) \\
\text{use }\ \psi(\vec{r}) &= \phi(\vec{r})e^{-iEt/\hbar} \\
E\phi(\vec{r}) &= -\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_x^2)\phi(\vec{r})
\end{aligned}
$$

To solve this we will use a technique called “separation of variables”.

Separation of Variables

$$
\begin{aligned}
\text{try }\ \phi(\vec{r}) &= \phi_x(x)\,\phi_y(y)\,\phi_z(z) \\
E\phi_x\,\phi_y\,\phi_z &= -\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_x^2)\phi_x\,\phi_y\,\phi_z \\
&= -\frac{\hbar^2}{2m}(\phi_y\,\phi_z\,\partial_x^2\phi_x + \phi_x\,\phi_z\,\partial_y^2\phi_y + \phi_x\,\phi_y\,\partial_z^2\phi_z) \\
&\quad \text{divide by }\ \phi(\vec{r}) = \phi_x\,\phi_y\,\phi_z \\
E &= -\frac{\hbar^2}{2m}\left(\frac{\partial_x^2\phi_x}{\phi_x} + \frac{\partial_y^2\phi_y}{\phi_y} + \frac{\partial_z^2\phi_z}{\phi_z}\right)
\end{aligned}
$$

With the equation rearranged like this into thee parts each of which only depends on one variable, we can simply solve 3 problems in 1D to get our 3D solution.

Separation of Variable, the magic:

$$
\begin{aligned}
\text{with } E &= E_x + E_y + E_z \\
\Rightarrow \quad E_x &= -\frac{\hbar^2}{2m}\frac{\partial_x^2 \phi_x}{\phi_x} \\
\Rightarrow \quad E_x \phi_x &= -\frac{\hbar^2}{2m}\partial_x^2 \phi_x \\
\Rightarrow \quad \partial_x^2 \phi_x &= -\frac{2m}{\hbar^2} E_x \phi_x \\
& \text{same for } y \text{ and } z
\end{aligned}
$$

Each of these problems individually is just our familiar 1D free particle, so we know the solutions...

Free Particle Solutions

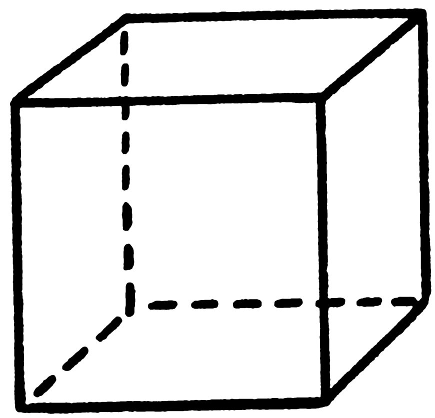
$$
\begin{aligned}
\phi_x = e^{ik_x x} \quad &, \quad \phi_y = e^{ik_y y} \;, \quad \phi_z = e^{ik_z z} \\
\text{with} \qquad & k_{x,y,z}^2 = \frac{2m}{\hbar^2} E_{x,y,z} \\
\text{such that} \qquad & E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2}{2m}\vec{k}^2 \\
\Rightarrow \psi(\vec{r}, t) \quad = \quad & \phi(\vec{r}) e^{-i\omega t} = e^{i(k_x x + k_y y + k_z z - \omega t)} \\
= \quad & e^{i(\vec{k}\cdot\vec{r} - \omega t)}
\end{aligned}
$$

Which is a wave propagating in the $\hat{k}$ direction. I hope it is clear now why I have been calling the e^{ikx} solutions in 1D "plane waves": when you recast them into 3D you get a wave in which there is no variation in the 2 dimensions perpendicular to the direction of propagation, just like a classical plane-wave from E&M.

5 Example: Infinite Square Well in 3D

The infinite square well is another of our friends from 1D that is easily generalized to 3D.

Infinite Square Well in 3D



This is a more realistic version of the "particle in a box" potential. For this example I'll assume that the box has length L on all sides,

3D Box Potential

$$V(\vec{r}) = \begin{cases} 0 & 0 < \{x, y, z\} < L \\ \infty & \text{else} \end{cases}$$

Since the potential is just zero in the region of interest, we can use separation of variables to solve this problem in the same way we did for the free particle. That is, the solution is just the product of three 1D solutions,

Recall: 1D Infinite Square Well EESs

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x)$$

$$\text{where} \qquad k_n = \frac{(n+1)\pi}{L} \quad \text{and} \quad E_n = \frac{\hbar^2}{2m}k^2$$

so that our energy eigenstates in 3D look like

3D Box EES

$$
\begin{aligned}
\phi_{\vec{n}}(\vec{r}) &= \left(\sqrt{\frac{2}{L}}\right)^3 \sin(k_x x)\sin(k_y y)\sin(k_z z) \\
\text{where} \qquad & k_{x,y,z} = \frac{(n_{x,y,z}+1)\pi}{L} \\
\Rightarrow E_{\vec{n}} &= \frac{\hbar^2}{2m}\vec{k}^2 \\
&= \frac{\hbar^2\pi^2}{2mL^2}\left[(n_x+1)^2+(n_y+1)^2+(n_z+1)^2\right]
\end{aligned}
$$

There are, however, some interesting features of the 3D solution that do not appear in 1D. First, the node-theorem and resulting guarantee of distinct energies for bound states no longer has any particular meaning. This means that we can easily create different energy eigenstates with the same energy eigenvalue.

Degeneracy

$$
\begin{aligned}
E_{0,0,0} &= 3E_0 \quad \text{where } E_0 = \frac{\hbar^2\pi^2}{2mL^2} \\
E_{1,0,0} &= E_{0,1,0} = E_{0,0,1} = 6E_0 \\
E_{2,1,0} &= E_{2,0,1} = E_{1,2,0} = \cdots = 14E_0 \\
&\vdots
\end{aligned}
$$

How would you remove the degeneracy of these energy eigenvalues? Try making the box sides different length, L_x, L_y, and L_z.

3D Non-Cubic Box EES

$$
E_{\vec{n}} = \frac{\hbar^2\pi^2}{2m}\left[\frac{(n_x+1)^2}{L_x^2}+\frac{(n_y+1)^2}{L_y^2}+\frac{(n_z+1)^2}{L_z^2}\right]
$$

By breaking the symmetry of the box, we have broken the degeneracy of the energy eigenstates.

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6 Example: Isotropic Oscillator

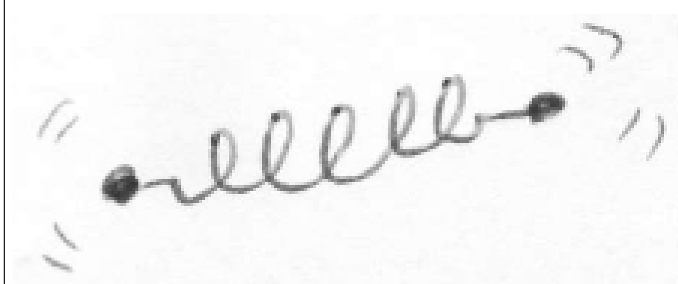
For another example, we can look at the 3D harmonic oscillator. We'll pick the easiest case in which the spring constant is the same in all directions, known as the "isotropic oscillator", so that

Isotropic Oscillator Potential

$$
\begin{aligned}
V(\vec{r}) &= \tfrac{1}{2}m\omega^2(x^2+y^2+z^2) \\
&\quad \text{or in spherical coordinates} \\
V(\vec{r}) &= \tfrac{1}{2}m\omega^2 r^2
\end{aligned}
$$

From this you might wonder why we don't use spherical coordinates, but we will get to that another day.

Diatomic Molecule



We will again use separation of variables, but it is a bit trickier here.

Separation of Variables

$$
\begin{aligned}
V(\vec{r}) &= V_x(x)+V_y(y)+V_z(z) \quad \text{where } V_x(x)=\tfrac{1}{2}m\omega^2x^2 \text{ etc.} \\
\text{use } \phi(\vec{r}) &= \phi_x(x)\,\phi_y(y)\,\phi_z(z) \\
E\phi_x\,\phi_y\,\phi_z &= \left[-\frac{\hbar^2}{2m}(\partial_x^2+\partial_y^2+\partial_x^2)+V_x+V_y+V_z\right]\phi_x\,\phi_y\,\phi_z \\
E &= -\frac{\hbar^2}{2m}\left(\frac{\partial_x^2\phi_x}{\phi_x}+\frac{\partial_y^2\phi_y}{\phi_y}+\frac{\partial_z^2\phi_z}{\phi_z}\right)+V_x+V_y+V_z
\end{aligned}
$$

Because the potential is separable into a sum of three parts, each of which depends only on one of our variables, we can again find 3 independent solutions and then add them together.

Separation of Variable, solve...

$$\begin{aligned} \text{with } E &= E_x + E_y + E_z \\ \Rightarrow \quad E_x &= -\frac{\hbar^2}{2m}\partial_x^2\phi_x + V_x \\ \Rightarrow \quad \partial_x^2\phi_x &= -\frac{2m}{\hbar^2}(E_x - \tfrac{1}{2}m\omega^2x^2)\phi_x \\ &\text{same for } y \text{ and } z \end{aligned}$$

This only works because $V(x)$ is separable into a sum of functions which each depend only on one coordinate!

Once again, our 1D solutions are all we need, since this is just the same 1D problem repeated 3 times. The energy eigenvalues are

Energies of Isotropic Oscillator

$$E_{\vec{n}} = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right)$$

The degeneracies are much worse in the case of the isotropic isolator than the 3D particle in a box.

Degeneracy

$$\begin{aligned} E_{0,0,0} &= \frac{3}{2}\hbar\omega && \times 1 \\ E_{1,0,0} = E_{0,1,0} = E_{0,0,1} &= \frac{5}{2}\hbar\omega && \times 3 \\ \underbrace{E_{1,1,0}}_{\times 3} = \underbrace{E_{2,0,0}}_{\times 3} &= \frac{7}{2}\hbar\omega && \times 6 \\ E_{1,1,1} = \underbrace{E_{2,1,0}}_{\times 6} = \underbrace{E_{3,0,0}}_{\times 3} &= \frac{9}{2}\hbar\omega && \times 10 \\ &\vdots \end{aligned}$$

Again, degeneracy arises from symmetry. If you make the resonant frequency different each direction, (i.e., $\omega_x \neq \omega_y \neq \omega_z$), you can break the symmetry and lift the degeneracy.

Energies of Non-Isotropic Oscillator

$$E_{\vec{n}} = \hbar\left[\omega_x(n_x + \tfrac{1}{2}) + \omega_y(n_y + \tfrac{1}{2}) + \omega_z(n_z + \tfrac{1}{2})\right]$$

7 Example: 2D QHO, 1D Infinite Square Well

It turns out that the laser cavities I work with on a regular basis are mathematically similar to a simple combination of the previous 2 cases: they are like a 2D QHO combined with a 1D infinite square well.

"Resonant Optical Cavity"

$$V(\vec{r}) = \begin{cases} \frac{1}{2}m\omega^2(x^2+y^2) & 0 < z < L \\ \infty & \text{else} \end{cases}$$

or in cylindrical coordinates

$$V(\vec{r}) = \begin{cases} \frac{1}{2}m\omega^2 r^2 & 0 < z < L \\ \infty & \text{else} \end{cases}$$

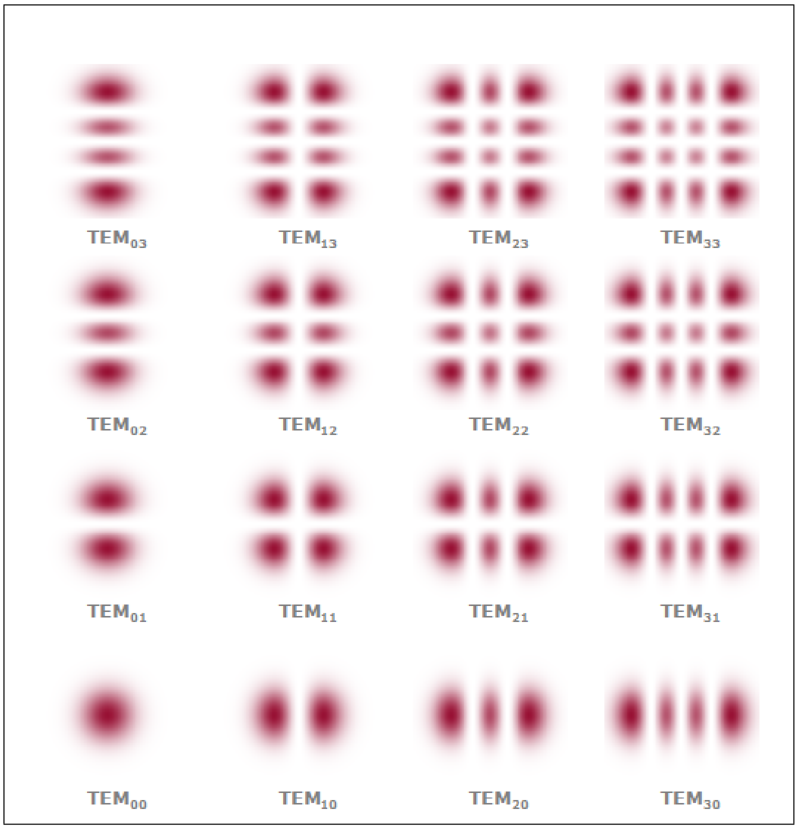
Again, separation of variables is successful here, and the energy eigenstates are products of the 1D solutions.

Energy Eigenstates

$$\phi_{\vec{n}}(\vec{r}) = \sqrt{\frac{2}{L}}\sin(k_z x)\, N_{nx}N_{ny}H_{nx}(x/\lambda)H_{ny}(y/\lambda)e^{-(x^2+y^2)/2\lambda^2}$$

$$E_{\vec{n}} = \hbar\omega(n_x+n_y+1) + \frac{\hbar^2\pi^2}{2mL^2}(n_z+1)^2$$

Since these solutions represent modes of a laser field propagating along the z axis, we see the 2D Hermite-Gaussian part of the solution as an intensity pattern if we point the beam at a CCD camera. They are labeled $TEM_{nx,ny}$, such that $TEM_{2,1}$ has 2 nodes in the x-direction and 1 node in the y-direction.



8 Next Time

- Spherically Symmetric Potentials
- Angular Momentum in Quantum Mechanics

9 Ehrenfest's Aside

A question about Ehrenfest's theorem was asked in lecture on Tuesday. Here is a quick answer:

Ehrenfest's theorem for some operator $\hat{A}$

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\left\langle [\hat{A}, \hat{E}] \right\rangle \tag{1}$$

... applied to the lowering operator $\hat{a}$, which is a bit strange since this operator does not represent an observable, but anyway...

Ehrenfest's theorem for $\hat{a}$

$$\begin{aligned} \frac{d\langle a\rangle}{dt} &= \frac{1}{i\hbar}\left\langle [\hat{a}, \hat{E}] \right\rangle \\ &= \frac{i}{\hbar}\left\langle [\hat{E}, \hat{a}] \right\rangle \\ &= -i\omega \langle a\rangle \end{aligned}$$

This suggests that the time dependence of $\langle a\rangle(t) = \langle\psi(x,t)|\hat{A}|\psi(x,t)\rangle$ can be factored out so that

$$\langle a\rangle(t) = \langle\psi(x,0)|\hat{A}|\psi(x,0)\rangle e^{-i\omega t} = \langle a\rangle_{t=0}\, e^{-i\omega t} \tag{2}$$

which pretty much just says that harmonic oscillators oscillate with angular frequency ω.