

Physics 486 Discussion 8 – 3D-Cartesian ; Momentum-Basis Operators

Time to move to **3D**! The Schrödinger equation gets the smallest of changes:

- position : the 1D position coordinate x becomes the 3D position vector $\vec{r} = \hat{x}x + \hat{y}y + \hat{z}z$.
- momentum : the 1D operator $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ becomes the 3D operator $\hat{p} = -i\hbar \vec{\nabla} = -i\hbar \left(\hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} \right)$

The Schrödinger equation therefore becomes

$$\hat{H} \Psi(\vec{r}) = \hat{E} \Psi(\vec{r}) \quad \text{where} \quad \hat{H} = \frac{|\vec{p}|^2}{2m} + V(\vec{r}) = -\frac{\hbar^2 \nabla^2}{2m} + V(\vec{r})$$

In Cartesian coordinates, the gradient and the Laplacian are

$$\vec{\nabla} = \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} \quad \text{and} \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad \text{respectively.}$$

Problem 1 : 3D Particle in a Box

Griffiths 4.2, Checkpoints 1

Use separation of variables in Cartesian coordinates to solve the infinite cubical well (or “particle in a box”):

$$V(x,y,z) = \begin{cases} 0 & \text{if } x, y, z \text{ are all between } 0 \text{ and } a \\ \infty & \text{otherwise} \end{cases}$$

- (a) Find the energy eigenstates $\psi(x,y,z)$ and the corresponding energies.
- (b) Call the distinct energies E_1, E_2, E_3, \dots , in order of increasing energy. Find the energies E_1 through E_6 .
- (c) Determine the degeneracies of the first 6 energies (i.e., find the number n_i of different states that share the same energy E_i).

FYI: In one dimension, degenerate bound states do not occur, but in three dimensions they are very common.

Problem 2 : Momentum-Basis Operators

adapted from Griffiths 3.12

We have learned that an x -dependent wavefunction $\psi_\alpha(x)$ is really a *representation* of a state $|\alpha\rangle$ in a *particular basis*, namely the basis of position eigenstates $|e_x\rangle$:

$$\boxed{\psi_\alpha(x) = \langle e_x | \alpha \rangle}$$

The wavefunction $\psi_\alpha(x) = \langle e_x | \alpha \rangle$ is the set of *coefficients* of the state $|\alpha\rangle$ along the basis elements $\{|e_x\rangle\}$, in the same way that (v_1, v_2, v_3) is the set of *coefficients* of the vector \vec{v} along the basis elements $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$.

► **IMPORTANT:** It is VITAL to realize that the state $|\alpha\rangle$ of a quantum system is NOT NECESSARILY AN EIGENFUNCTION OF ANYTHING. It can always be written as a SUPERPOSITION OF EIGENSTATES of some Hermitian operator(s), but is not necessarily in a *single* eigenstate of *any* operator. Since we spend so much time determining energy eigenstates, and since we are so used to energy being a constant in classical mechanics, it is a particularly common misconception that a system must always be in an energy eigenstate ... but that is ABSOLUTELY NOT TRUE. Think of the most realistic representation we have seen of a moving free electron : the moving Gaussian wave packet. That wave packet was *concentrated* at a particular

¹ **Q1 (a)** $\psi(x,y,z) = (2/a)^{3/2} \sin(n_x \pi x/a) \sin(n_y \pi y/a) \sin(n_z \pi z/a)$, $E = \pi^2 \hbar^2 (n_x^2 + n_y^2 + n_z^2) / (2ma^2)$ for $n_x, n_y, n_z = 1, 2, 3, \dots$
(b) $E_{\{1,2,3,4,5,6\}} = \pi^2 \hbar^2 / (2ma^2) \cdot \{3, 6, 9, 11, 12, 14\}$ **(c)** degeneracies $d_{\{1,2,3,4,5,6\}} = \{1, 3, 3, 3, 1, 6\}$

momentum, and therefore energy, but its Fourier transform was also a Gaussian, indicating that it was spread across many momenta, and therefore many energies.

(a) **We did this part in lecture today; do (a) to get caught up if you missed lecture.**

We can build different wavefunctions to represent a state $|\alpha\rangle$ by projecting it onto different bases.

Specifically, we can build a wavefunction $\psi_\alpha(q)$ in the eigenspace $\{|e_q\rangle\}$ of any Hermitian operator Q , since Hermitian operators always have complete eigenspaces. In class we concentrated on transforming wavefunctions from position-basis to momentum-basis. Show that the general rule to transform of an x -basis wavefunction $\psi(x)$ to a q -basis wavefunction $\phi(q)$ describing the same state is :

$$\boxed{\phi(q) = \int \psi_q^*(x) \psi(x) dx} \quad \text{where } \{q\} \text{ are the eigenvalues of a Hermitian operator } Q, \text{ and } \psi_q(x) \text{ denotes the eigenfunction of } Q \text{ with eigenvalue } q.$$

► STRATEGY: Go to Dirac notation straight away, and make good use of the completeness relation

$$\sum_y |e_y\rangle\langle e_y| = 1 \text{ for a discrete set of eigenvalues } \{y\} \quad \text{or} \quad \int dy |e_y\rangle\langle e_y| = 1 \text{ for a continuous set .}$$

► IMPORTANT : Recall that this basis-switching is not just a mathematical curiosity; the *extreme* usefulness of changing the basis of a wavefunction $\psi(x)$ is that $\psi(x)^*\psi(x)$ gives you the **probability density** $P(x)$ of finding the system at position x ... and so $\phi(q)^*\phi(q)$ gives you the probability density $P(q)$ of finding it at the eigenvalue q of **any other observable** Q : i.e.

$$\boxed{P(q) = |\langle e_q | \alpha \rangle|^2 = |\phi_\alpha(q)|^2}$$

as we wrote down last week. No longer are we constrained to simply obtain the expectation value $\langle Q \rangle$ and variances $\langle Q^2 \rangle$ from a quantum wavefunction, we can now obtain complete probability distributions for any observable Q .

(b) In the position basis, the operators for position x , momentum p , and any dynamical property $Q(x, p)$ are :

$$\hat{x} = x, \quad \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad \hat{Q} = Q\left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}\right).$$

What are the corresponding operators in the momentum-basis, i.e. with p as the independent variable instead of x ? The operator for momentum itself is clearly just p , but what is the p -dependent operator for x ? What a mind-bending question! ☺ It turns out the answer is

$$\hat{p} = p, \quad \hat{x} = -\frac{\hbar}{i} \frac{\partial}{\partial p}, \quad \hat{Q} = Q\left(-\frac{\hbar}{i} \frac{\partial}{\partial p}, x\right)$$

Where did that \hat{x} come from?? To show that the position operator in momentum space is indeed the one given above, prove that the expectation value of position is

$$\langle x \rangle = \int \Phi^*(p) \left(-\frac{\hbar}{i} \frac{\partial}{\partial p}\right) \Phi(p) dp$$

HINT #1: Start with the formula you *know* for $\langle x \rangle$.

HINT #2 : Notice that $x \exp(ipx / \hbar) = -i\hbar(d / dp) \exp(ipx / \hbar)$.

► FYI: In principle, you can do *all* calculations in momentum space instead of position space (though not always as easily). It is an interesting mental exercise to look at the quantum world as if p , not x , is the independent variable for your wavefunctions i.e. the basis in which you *think*. Try viewing the world through momentum-coloured glasses. 8-)