PH423 Assignment 1

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August 25, 2020

1. Prove that matrix elements of the momentum operator in position space take the form

$$\langle x| \hat{\mathbf{P}} |x'\rangle = -\imath\hbar \frac{\mathrm{d}}{\mathrm{d}x} \delta(x - x') \ .$$

We consider the action of the commutator $\left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right]$ on an arbitrary state ϕ,

$$\left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right] \phi(x) \ . \tag{1}$$

Starting with equation 1, we first write it in bra-ket notation as

$$\left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right] \phi(x) = \langle x| \left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right] |\phi\rangle \ . \tag{2}$$

Since $\left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right] = \imath\hbar$, we get

$$\langle x| \left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right] |\phi\rangle = \langle x| \imath\hbar |\phi\rangle \ . \tag{3}$$

On either side, we can introduce the identity operator as $\left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right] \cdot \hat{\mathbf{1}}$ and $\imath\hbar \cdot \hat{\mathbf{1}}$, and use the position space completeness relation $\int \mathrm{d}x' \, |x'\rangle\langle x'| = \hat{\mathbf{1}}$ to obtain

$$\int \mathrm{d}x' \, \langle x| \left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right] |x'\rangle \langle x'|\phi\rangle = \int \mathrm{d}x' \, \langle x| \imath\hbar |x'\rangle \langle x'|\phi\rangle \ . \tag{4}$$

Expanding the commutator operation $\langle x| \left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right] |x'\rangle$ as

$$\langle x| \left[\hat{\mathbf{X}}, \hat{\mathbf{P}}\right] |x'\rangle = \langle x| \hat{\mathbf{X}}\hat{\mathbf{P}} |x'\rangle - \langle x| \hat{\mathbf{P}}\hat{\mathbf{X}} |x'\rangle$$

and applying the action of $\hat{\mathbf{X}}$ on $|x'\rangle$ and $\langle x|$, we obtain

$$\int \mathrm{d}x' \, (x - x') \langle x| \hat{\mathbf{P}} |x'\rangle \langle x'|\phi\rangle = \int \mathrm{d}x' \, \langle x| \imath\hbar |x'\rangle \langle x'|\phi\rangle \ . \tag{5}$$

Since the state $\phi(x)$ chosen was arbitrary, we get the weak equivalence

$$(x - x') \langle x| \hat{\mathbf{P}} |x'\rangle = \iota\hbar \langle x|x'\rangle \ . \tag{6}$$

We know $\langle x|x'\rangle = \delta(x - x')$, and using

$$\delta(x) = -x\delta'(x)$$

we get

$$(x - x') \langle x| \hat{\mathbf{P}} |x'\rangle = -\iota\hbar(x - x')\frac{\mathrm{d}}{\mathrm{d}x}\delta(x - x') \ . \tag{7}$$

And finally, dividing both sides by $(x - x')$, assuming $x \neq x'$, we get the required matrix element

$$\langle x| \hat{\mathbf{P}} |x'\rangle = -\iota\hbar\frac{\mathrm{d}}{\mathrm{d}x}\delta(x - x') \ . \tag{8}$$

□

2. Starting from the abstract ket form of the Schrodinger eqn. derive the Schrodinger eqn. in the co-ordinate basis

The Schrodinger eqn. in the abstract ket form is given as

$$\hat{\mathbf{H}} \ |\psi\rangle = E \ |\psi\rangle \ . \tag{9}$$

In the position basis, $\hat{\mathbf{H}}$ can be expressed in the form of a matrix, while $|\psi\rangle$ can be expressed in terms of components in the basis. In the position basis, the components of $|\psi\rangle$ form the wavefunction

$$\langle x|\psi\rangle = \psi(x) \ . \tag{10}$$

The Hamiltonian becomes a matrix in the position basis, with components given by

$$H_{xy} = \langle x| \hat{\mathbf{H}} |y\rangle \ . \tag{11}$$

Applying this to equation 9. We multiply by $\langle x|$ on the left side and insert an identity on the right hand side. The identity is given by

$$\hat{\mathbf{1}} = \int dy \ |y\rangle \langle y| \tag{12}$$

So, now we obtain

$$\int dy \ \langle x| \hat{\mathbf{H}} |y\rangle \langle y|\psi\rangle = E \langle x|\psi\rangle \ . \tag{13}$$

Simplifying to components, we get

$$\int dy\, H_{xy}\psi(y) = E\,\psi(x) \tag{14}$$

and now our components are

$$H_{xy} = -\frac{\hbar^2}{2m}\delta''(x-y) + V\,\delta(x-y)\ . \tag{15}$$

We plug this in to equation 14. We get

$$\int dy\,[-\frac{\hbar^2}{2m}\delta''(x-y)\psi(y)] + \int dy\,V\,\psi(y)\delta(x-y) = E\,\psi(x)\ , \tag{16}$$

$$-\frac{\hbar^2}{2m}\int dy\,\delta''(x-y)\psi(y) + V\,\psi(x) = E\,\psi(x)\ . \tag{17}$$

Using Integration by Parts on the integral twice, we obtain

$$-\frac{\hbar^2}{2m}\int dy\,\delta(x-y)\psi''(y) + V\,\psi(x) = E\,\psi(x)\ , \tag{18}$$

$$-\frac{\hbar^2}{2m}\psi''(x) + V\,\psi(x) = E\,\psi(x)\ . \tag{19}$$

Upon generalising this a bit, we get

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi\ . \tag{20}$$

This is quite obviously, our Schrodinger's Equation in co-ordinate form.

3. Calculate the matrix elements of the time-evolution operator, i.e. the propagator, in position space.

We use the identity $\int_{-\infty}^{+\infty} |p\rangle\langle p|\, dp = \hat{\mathbf{1}}$ to get:

$$\langle x|\,U(t)\,|x'\rangle = \int_{-\infty}^{+\infty} \langle x|p\rangle\,\langle p|x'\rangle\, e^{-ip^2t/2m\hbar}dp\ . \tag{21}$$

We use the representation of momentum eigenvectors in the position basis to obtain

$$\langle x|\,U(t)\,|x'\rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} e^{ip(x-x')/\hbar}\times e^{-ip^2t/2m\hbar}dp\ . \tag{22}$$

Finally, we integrate the resulting Gaussian to obtain the result,

$$\langle x|\,U(t)\,|x'\rangle = (\frac{m}{2\pi\hbar i t})^{1/2}e^{im(x-x')^2/2\hbar t}\ . \tag{23}$$