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Program Studi S2 Pendidikan Fisika

FAKULTAS KEGURUAN DAN ILMU PENDIDIKAN
UNIVERSITAS SEBELAS MARET (UNS) SURAKARTA

e Learning :

The Expansion Postulate and Operator Methods in Quantum Mechanics

Pertemuan ke-11 :
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1. Interpretation of The Expansion Coeffisients

Fourier's theorem states that any function $\psi(x)$ that satisfies the boundary conditions $\psi(0) = \psi(a) = 0$ can be written in the form

$$\psi(x) = \sum_{n=1}^{\infty} C_n \sin \frac{n\pi x}{a} \tag{3-29}$$

Since the eigenfunctions of H for the infinite well are proportional to $\sin n\pi x/a$, we write the preceding expression in terms of the eigenfunctions $u_n(x)$:

$$\psi(x) = \sum_{n=1}^{\infty} A_n u_n(x) \tag{3-30}$$

The orthonormality relation (3-23) can be used to find A_n. We see that

$$\int_0^a dx\, u_m^*(x)\psi(x) = \int_0^a dx\, u_m^*(x) \sum_{n=1}^{\infty} A_n u_n(x)$$

$$= \sum_{n=1}^{\infty} A_n \int_0^a dx\, u_m^*(x) u_n(x) = \sum_{n=1}^{\infty} A_n \delta_{mn} = A_m$$

Interpretation of The Expansion Coeffisients…

so that

$$A_m = \int_0^a dx\, u_m^*(x)\psi(x) \tag{3-31}$$

As in our discussion of the free wave packet, we can calculate the time development of this arbitrary initial wave function $\psi(x)$. Since each of the eigenfunctions $u_n(x)$ acquires its own time dependence $e^{-iE_nt/\hbar}$, we have quite generally

$$\psi(x, t) = \sum A_n u_n(x) e^{-iE_nt/\hbar} \tag{3-32}$$

Interpretation of The Expansion Coeffisients…

To interpret the coefficients A_n we calculate the expectation value of the energy in an arbitrary state $\psi(x)$. Since inside the box $H = p^2/2m$, and outside the box $\psi(x) = 0$, and since

$$Hu_n(x) = E_n u_n(x)$$

It follows that

$$\begin{aligned}\langle H \rangle = \int_0^a dx\, \psi^*(x) H \psi(x) &= \int_0^a dx\, \psi^*(x) H \sum_n A_n u_n(x) \\ &= \sum_n A_n \int_0^a dx\, \psi^*(x) E_n u_n(x) \qquad (3\text{-}33) \\ &= \sum_n E_n |A_n|^2\end{aligned}$$

We also note that

$$\int_0^a dx\, \psi^*(x)\psi(x) = 1 \qquad (3\text{-}34)$$

Interpretation of The Expansion Coeffisients…

implies that

$$1 = \int_0^a dx\, \psi^*(x) \sum_n A_n u_n(x) = \sum_n A_n A_n^* = \sum_n |A_n|^2 \qquad (3\text{-}35)$$

Comparison with (3-33) and (3-35) immediately suggests that $|A_n|^2$, where

$$A_n = \int_0^a dx\, u_n^*(x)\psi(x) \qquad (3\text{-}36)$$

be interpreted as *the probability that a measurement of the energy for the state $\psi(x)$ yields the eigenvalue E_n.*

2. Operators in The Schrodinger Equation

How do we get to the Schrödinger equation from our abstract framework? Consider the harmonic oscillator problem. Starting from (6-42), we get

$$\langle x|A|0\rangle = 0 \tag{6-50}$$

The original definition of A then implies that

$$\left\langle x\left|\sqrt{\frac{m\omega}{2\hbar}}\,x_{\mathrm{op}} + i\sqrt{\frac{1}{2m\omega\hbar}}\,p_{\mathrm{op}}\right|0\right\rangle = 0 \tag{6-51}$$

Operators in The Schrodinger Equation…

We now use

$$\langle x|x_{op}|0\rangle = x\langle x|0\rangle \tag{6-52}$$

and

$$\begin{aligned}\langle x|p_{op}|0\rangle &= \int_{-\infty}^{\infty} dp\langle x|p_{op}|p\rangle\langle p|0\rangle = \int_{-\infty}^{\infty} dp\, p\langle x|p\rangle\langle p|0\rangle \\ &= \int_{-\infty}^{\infty} dp\, p\, \frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}\langle p|0\rangle = \frac{\hbar}{i}\frac{d}{dx}\int_{-\infty}^{\infty} dp\, \frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}\langle p|0\rangle \\ &= \frac{\hbar}{i}\frac{d}{dx}\int_{-\infty}^{\infty} dp\langle x|p\rangle\langle p|0\rangle = \frac{\hbar}{i}\frac{d}{dx}\langle x|0\rangle\end{aligned} \tag{6-53}$$

We now denote $\langle x|0\rangle$ by $u_0(x)$, the ground-state wave function. Equation (6-50) now becomes a differential equation in x-space, which reads (after a little algebra)

Operators in The Schrodinger Equation…

This is a simple differential equation, whose solution is

$$u_0(x) = Ce^{-m\omega x^2/2\hbar} \tag{6-55}$$

The constant C is determined by the normalization requirement that

$$1 = C^2 \int_{-\infty}^{\infty} dx\, e^{-m\omega x^2/\hbar} = C^2 \sqrt{\frac{\hbar\pi}{m\omega}} \tag{6-56}$$

so that

$$C = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \tag{6-57}$$

We may also obtain the higher energy states by working out in detail

$$\begin{aligned} u_n(x) &= \frac{1}{\sqrt{n!}}(A^+)^n u_0(x) \\ &= \frac{1}{\sqrt{n!}}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\left(\sqrt{\frac{m\omega}{2\hbar}}\,x - \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)^n e^{-m\omega x^2/2\hbar} \end{aligned} \tag{6-58}$$

Operators in The Schrodinger Equation…

In a general Schrödinger equation in which $H = \frac{p_{op}^2}{2m} + V(x_{op})$, we have

$$\langle x|V(x_{op})|E\rangle = V(x)\langle x|E\rangle \tag{6-59}$$

To get $\langle x|p_{op}|E\rangle$ we calculate

$$\begin{aligned}\langle x|p_{op}|E\rangle &= \int_{-\infty}^{\infty} dp\langle x|p_{op}|p\rangle\langle p|E\rangle = \int_{-\infty}^{\infty} dp\, p\langle x|p\rangle\langle p|E\rangle \\ &= \frac{\hbar}{i}\frac{d}{dx}\langle x|E\rangle\end{aligned} \tag{6-60}$$

by following the same steps that led to (6-53). From this we see that

$$\langle x|H|E\rangle = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\langle x|E\rangle + V(x)\langle x|E\rangle = E\langle x|E\rangle \tag{6-61}$$

which is just the Schrödinger energy eigenvalue equation!

3. The Time Dependence of Operators

We conclude this chapter by discussing the time development of a system in our representation-independent way. The equation that describes the evolution of a system is the time-dependent Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle \tag{6-62}$$

This is now an operator equation in an abstract space. $|\psi(t)\rangle$ is a vector in that space and it points in a direction that depends on time. The solution of this equation is

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle \tag{6-63}$$

where $|\psi(0)\rangle$ is the vector at time $t = 0$. The operator in front is defined by

$$e^{-iHt/\hbar} = \sum_{n=0}^{\infty} \frac{1}{n!}(-iHt/\hbar)^n \tag{6-64}$$

The Time Dependence of Operators…

The solution (6-63) allows us to describe the change with time of the expectation value of any operator B that does not have any explicit time dependence:

$$\begin{aligned}\langle B\rangle_t &= \langle\psi(t)|B|\psi(t)\rangle \\ &= \langle e^{-iHt/\hbar}\psi(0)|B|e^{-iHt/\hbar}\psi(0)\rangle \\ &= \langle\psi(0)|e^{iHt/\hbar}Be^{-iHt/\hbar}|\psi(0)\rangle \\ &= \langle\psi(0)|B(t)|\psi(0)\rangle\end{aligned} \tag{6-65}$$

where we have defined

$$B(t) = e^{iHt/\hbar}Be^{-iHt/\hbar} \tag{6-66}$$

$$\begin{aligned}\frac{d}{dt}B(t) &= \frac{i}{\hbar}He^{iHt/\hbar}Be^{-iHt/\hbar} - \frac{i}{\hbar}e^{iHt/\hbar}Be^{-iHt/\hbar}H \\ &= \frac{i}{\hbar}(HB(t) - B(t)H) = \frac{i}{\hbar}[H, B(t)]\end{aligned} \tag{6-67}$$

The Time Dependence of Operators…

For the harmonic oscillator

$$H = \hbar\omega(A^{+}A + \tfrac{1}{2}) \tag{6-68}$$

and since H is a constant of the motion, we have

$$H = \hbar\omega(A^{+}(t)A(t) + \tfrac{1}{2}) \tag{6-69}$$

We can also show, using (6-66), that

$$[A(t), A^{+}(t)] = 1 \tag{6-70}$$

Eq. (6-67) implies that

$$\begin{aligned} \frac{d}{dt}A(t) &= -i\omega A(t) \\ \frac{d}{dt}A^{+}(t) &= i\omega A^{+}(t) \end{aligned} \tag{6-71}$$

The Time Dependence of Operators…

whose solutions are

$$
\begin{aligned}
A(t) &= e^{-i\omega t}A(0) \\
A^{+}(t) &= e^{i\omega t}A^{+}(0)
\end{aligned}
\tag{6-72}
$$

We may use these to express the operators $p(t)$ and $x(t)$ in terms of $p(0)$ and $x(0)$:

$$
\begin{aligned}
p(t) &= p(0)\ \cos\ \omega t - m\omega x(0)\ \sin\ \omega t \\
x(t) &= x(0)\ \cos\ \omega t + \frac{p(0)}{m\omega}\ \sin\ \omega t
\end{aligned}
\tag{6-73}
$$

Note that in the Heisenberg picture we only deal with operators. We have therefore omitted the subscript *op* to avoid cluttering up the equations.

Exercises: (at paper),

1. Use the general operator equation (6-53) to Calculate $\langle n|x^2|n\rangle$ and $\langle n|p^2|n\rangle$.

$$x = \sqrt{\frac{\hbar}{2m\omega}}(A + A^+)$$

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(A^+ - A)$$

2. Use the general operator equation of motion (6-67) to solve for the time dependence of the operator $x(t)$ given that

$$H = \frac{p^2(t)}{2m} + mgx(t)$$

Thank you