MPF1204, FISIKA KUANTUM (3 SKS)
Program Studi S2 Pendidikan Fisika

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

e Learning :

THE GENERAL STRUCTURE OF WAVE MECHANICS

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DR. Suharno, M.Si

1. The Hamiltonian Operator

The Hamiltonian Operator

The time dependence of the wave function is given by

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = H\psi(x, t) \tag{5-1}$$

On the right side of the equation the wave function is acted upon by an *operator H*, the Hamiltonian, which, because it governs the time development of the system, plays a central role in quantum mechanics. For a single particle moving in a potential $V(x)$, it is an operator version of the total energy

$$H = \frac{p_{op}^2}{2m} + V(x) \tag{5-2}$$

where the momentum is represented by its operator version

$$p_{op} = -i\hbar \frac{\partial}{\partial x} \tag{5-3}$$

The Hamiltonian Operator …

If $V(x)$ has no explicit time dependence, then (5-1) can be partially solved by writing

$$\psi(x, t) = u_E(x)e^{-iEt/\hbar} \tag{5-4}$$

The function $u_E(x)$ is a solution of the differential equation

$$Hu_E(x) = Eu_E(x) \tag{5-5}$$

Some properties of eigenvalues and eigenfunctions are familiar from our examples in Chapter 3.

1. Eigenfunctions that correspond to different eigenvalues are *orthogonal*; that is,

$$\int_{-\infty}^{\infty} dx\, u_{E_1}^*(x)u_{E_2}(x) = 0 \tag{5-6}$$

when $E_1 \neq E_2$.

The Hamiltonian Operator …

2. The eigenfunctions of H form a complete set. By this we mean the following: Any *arbitrary* square integrable function of x, one that satisfies

$$\int_{-\infty}^{\infty} dx|\psi(x)|^2 < \infty$$

may be expanded in terms of eigenfunctions of H, so that

$$\psi(x) = \sum_E C_E u_E(x) \tag{5-7}$$

where the sum is over *all* the eigenfunctions. The eigenvalues of H, the *spectrum of H*, may be a discrete set as in the infinite box, or it may involve discrete values (labeled by n as for the well) and also as a continuous energy variable, as appears in the example of a plane wave traversing a potential well seen in Chapter 4. In that latter case we have the schematic expression

$$\psi(x) = \sum_n C_n u_n(x) + \int dE C(E) u_E(x) \tag{5-8}$$

The Hamiltonian Operator …

3. The eigenfunctions can be multiplied by constants so that they become *normalized*. For the discrete set this reads

$$\int_{-\infty}^{\infty} dx\, u_m^*(x) u_n(x) = \delta_{mn} \qquad (5\text{-}9)$$

4. Consider any solution of (5-1), $\psi(x, t)$. At $t = 0$, the wave function $\psi(x, 0)$, which we write as $\psi(x)$, may be expanded as in (5-7), for example. Because each eigenfunction has a simple time dependence given by $e^{-iEt/\hbar}$, the time-dependent solution has the form

$$\psi(x, t) = \sum_E C_E u_E(x) e^{-iEt/\hbar} \qquad (5\text{-}10)$$

2. Time Dependence and The Classical Limit

Let us now turn to the important question of the classical limit of quantum theory. To do this we must first study the time development of expectation values of operators. In general, the expectation value of an operator changes with time. It may change with time because the operator has an explicit time dependence—for example, the operator $x + pt/m$—and it also changes with time because the expectation value is taken with respect to a wave function that itself changes with time. If we write

$$\langle A \rangle_t = \int \psi^*(x, t)\, A\psi(x, t)\, dx \tag{5-48}$$

Time Dependence and The Classical Limit…

then

$$\frac{d}{dt}\langle A\rangle_t = \int \psi^*(x,t)\,\frac{\partial A}{\partial t}\,\psi(x,t)\,dx$$
$$+\int \frac{\partial \psi^*(x,t)}{\partial t}\,A\psi(x,t)\,dx$$
$$+\int \psi^*(x,t)\,A\,\frac{\partial \psi(x,t)}{\partial t}\,dx$$
$$=\left\langle\frac{\partial A}{\partial t}\right\rangle_t+\int\left(\frac{1}{i\hbar}H\psi(x,t)\right)^* A\psi(x,t)$$
$$+\int \psi^*(x,t)\,A\left(\frac{1}{i\hbar}H\psi(x,t)\right)$$
$$=\left\langle\frac{\partial A}{\partial t}\right\rangle_t+\frac{i}{\hbar}\int \psi^*(x,t)\,HA\psi(x,t)\,dx$$
$$-\frac{i}{\hbar}\int \psi^*(x,t)\,AH\psi(x,t)\,dx$$

Time Dependence and The Classical Limit…

that is,

$$\frac{d}{dt}\langle A\rangle_t = \left\langle \frac{\partial A}{\partial t} \right\rangle_t + \frac{i}{\hbar}\langle [H, A]\rangle_t \tag{5-49}$$

In the derivation we made use of the fact that H is a hermitian operator. We observe that if A has no explicit time dependence, then the change of the expectation value *for any state* is

$$\frac{d}{dt}\langle A\rangle_t = \frac{i}{\hbar}\langle [H, A]\rangle_t \tag{5-50}$$

Time Dependence and The Classical Limit…

If the operator commutes with H, then its expectation value is always constant; that is, we may say that *the observable is a constant of the motion*. If the Hamiltonian is one of the complete set of commuting observables, then all the others are constants of the motion.

Let us consider successively $A = x$ and $A = p$. We first have

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle [H, x]\rangle$$
$$= \frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m} + V(x), x\right]\right\rangle$$

Now x commutes with any function of x,

$$[V(x), x] = 0 \qquad (5\text{-}51)$$

so that we only have to calculate

$$[p^2, x] = p[p, x] + [p, x]p$$
$$= \frac{2\hbar}{i}p \qquad (5\text{-}52)$$

Time Dependence and The Classical Limit…

Thus we obtain

$$\frac{d}{dt}\langle x\rangle = \left\langle \frac{p}{m}\right\rangle \tag{5-53}$$

Next we have

$$\begin{aligned}\frac{d}{dt}\langle p\rangle &= \frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m} + V(x), p\right]\right\rangle \\ &= -\frac{i}{\hbar}\langle[p, V(x)]\rangle\end{aligned} \tag{5-54}$$

since p^2 and p evidently commute. To evaluate the last commutator, we note that

$$\begin{aligned}pV(x)\,\psi(x) - V(x)\,p\psi(x) &= \frac{\hbar}{i}\frac{d}{dx}[V(x)\,\psi(x)] - \frac{\hbar}{i}V(x)\frac{d}{dx}\psi(x) \\ &= \frac{\hbar}{i}\frac{dV(x)}{dx}\psi(x)\end{aligned} \tag{5-55}$$

Time Dependence and The Classical Limit…

so that

$$[p, V(x)] = \frac{\hbar}{i}\frac{dV(x)}{dx} \tag{5-56}$$

and thus

$$\frac{d}{dt}\langle p\rangle_t = -\left\langle \frac{dV(x)}{dx} \right\rangle_t \tag{5-57}$$

We may combine (5-53) and (5-57) to obtain

$$m\frac{d^2}{dt^2}\langle x\rangle_t = -\left\langle \frac{dV(x)}{dx} \right\rangle_t \tag{5-58}$$

Time Dependence and The Classical Limit…

which looks very much like the equation of motion of a classical point particle in a potential $V(x)$

$$m\frac{d^2x_{cl}}{dt^2} = -\frac{dV(x_{cl})}{dx_{cl}} \tag{5-59}$$

The only thing that keeps us from making the identification

$$x_{cl} = \langle x \rangle \tag{5-60}$$

is that

$$\left\langle \frac{dV}{dx} \right\rangle \neq \frac{d}{d\langle x \rangle} V(\langle x \rangle) \tag{5-61}$$

Under the circumstances where the preceding inequality becomes an approximate equality, the motion is essentially classical, as was first noted by Ehrenfest. This requires that the potential be a slowly varying function of its argument. If we write

$$F(x) = -\frac{dV(x)}{dx} \tag{5-62}$$

Exercises/Homework (at a paper),

THE GENERAL STRUCTURE OF WAVE MECHANICS

Exercises/homework:

1. Use the commutation relations between the operators x and p to obtain the equations describing the time dependence of $\langle x \rangle$ and $\langle p \rangle$ for the Hamiltonian given by

$$H = \frac{p^2}{2m} + \frac{1}{2} m(\omega_1^2 x^2 + \omega_2 x + C)$$

Solve the equations of motion you obtained in Problem [redacted]. Write your solutions in terms of $\langle x \rangle_0$ and $\langle p \rangle_0$, the expectation values at time $t = 0$.

2. An electron in an oscillating electric field is described by the Hamiltonian operator

$$H = \frac{p^2}{2m} - (eE_o \cos\omega t)x$$

Calculate expressions for the time dependence of $\langle x \rangle$, $\langle p \rangle$, and $\langle H \rangle$.

Solve the equations of motion you obtained in Problem [redacted]. Write your solutions in terms of $\langle x \rangle_0$ and $\langle p \rangle_0$, the expectation values at time $t = 0$.

Thank you