DETERMINATE STATES

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Section 3.2.2; Problem 3.6.

A *determinate state* is a state in which an observable quantity has a definite value or, to put it another way, if a measurement of this quantity is done, only one possible value can be found.

If the hermitian operator corresponding to this observable is $\hat{Q}$, and the observed value is q, we must have

$$\left\langle \Psi | \hat{Q}\Psi \right\rangle = q \tag{1}$$

This equation tells us only that the average value obtained in a measurement is q; it doesn't constrain q to be a single value. However, the determinacy condition also means that the variance of the observable must be zero (since there is only one possible outcome of a measurement). This means

$$\begin{aligned} \left\langle \Psi \middle| \left(\hat{Q}-q\right)^2 \Psi \right\rangle &= 0 & (2)\\ \left\langle \left(\hat{Q}-q\right)\Psi \middle| \left(\hat{Q}-q\right)\Psi \right\rangle &= 0 & (3) \end{aligned}$$

This means that the function $\left(\hat{Q}-q\right)\Psi$ itself must be zero (since the inner product of a function with itself is strictly non-negative). Thus we get the condition

$$\hat{Q}\Psi = q\Psi \tag{4}$$

This is an *eigenvalue* equation, with q being the eigenvalue of the operator $\hat{Q}$, and Ψ being the corresponding *eigenfunction*. (The prefix 'eigen' is German for 'self'.)

The Schrödinger equation for stationary states is itself an eigenvalue equation, as we can write it as

$$\hat{H}\Psi = E\Psi \tag{5}$$

where $\hat{H}$ is the hamiltonian operator and E is the energy. The wave function corresponding to E is the eigenfunction.

Another example is that of a periodic function $f(\phi)$ which has the property

$$f(\phi+2\pi)=f(\phi) \tag{6}$$

We'll consider the operator $d^2/d\phi^2$ and find its eigenvalues and eigenfunctions. We can use the same technique as we used for the hamiltonian to show that this operator is hermitian. The difference here is that the domain of the function is $[0,2\pi]$ rather than infinite, so integrals have the ends of this domain as limits.

$$\begin{aligned}
\langle f|f''\rangle &= \int_0^{2\pi} f^* f'' d\phi && (7)\\
&= f^* f'\Big|_0^{2\pi} - \int_0^{2\pi} (f^*)' f' d\phi && (8)\\
&= -(f^*)' f\Big|_0^{2\pi} + \int_0^{2\pi} (f^*)'' f d\phi && (9)\\
&= \langle f''|f\rangle && (10)
\end{aligned}$$

At each stage, we've thrown away the integrated terms since, due to the function's periodicity, the values of $f(\phi)$ and $f'(\phi)$ are the same at 0 and 2π.

It's a bit easier to solve the eigenvalue equation if we write it as

$$\frac{d^2 f}{d\phi^2}=q^2 f \tag{11}$$

This has two linearly independent solutions:

$$\begin{aligned}
f_1 &= e^{q\phi} && (12)\\
f_2 &= e^{-q\phi} && (13)
\end{aligned}$$

The periodicity condition requires that

$$\begin{aligned}
f_1(0) &= f_1(2\pi) && (14)\\
1 &= e^{2\pi q} && (15)
\end{aligned}$$

From this, we see that q must be imaginary, and is restricted to

$$q=ni \tag{16}$$

for some integer (positive, negative or zero) n. The periodic constraint on $f_2(\phi)$ leads to the same result for q.

Thus the eigenvalues are all negative squares:

$$q^2 = 0, -1, -4, -9, \ldots - n^2, \ldots \tag{17}$$

For each eigenvalue (except 0), there are two linearly independent eigenfunctions, so in this case the system is degenerate.

PINGBACKS

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