Chapter 8
Problems in Two and Three-Dimensions: General Considerations

8.1 Separable Hamiltonians in x, y, z

Going from one to two or three dimensions significantly increases the difficulty of solving Schrödinger's equation. In general the problem must be solved numerically. Moreover, the numerical solutions may be difficult to obtain. However there are classes of *separable* potentials for which the solution can be obtained easily. If the classical potential can be written as

$$V(x, y, z) = V_x(x) + V_y(y) + V_z(z), \tag{8.1}$$

then the corresponding quantum Hamiltonian for a particle having mass m moving in this potential is

$$\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z, \tag{8.2}$$

where

$$\hat{H}_j = \frac{\hat{p}_j^2}{2m} + \hat{V}_j; \quad j = x, y, z. \tag{8.3}$$

The eigenfunctions of $\hat{H}$ are simply the products of the eigenfunctions of $\hat{H}_x$ and $\hat{H}_y$ and $\hat{H}_z$,

$$\psi_E(x, y, z) = \psi_{E_x}(x)\,\psi_{E_y}(y)\,\psi_{E_z}(z), \tag{8.4}$$

provided

$$E = E_x + E_y + E_z, \tag{8.5}$$

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where $\psi_{E_j}(j)$ is an eigenfunction of $\hat{H}_j$ and E_j an eigenenergy of $\hat{H}_j$ $(j = x, y, z)$. You can convince yourselves that the trial solution (8.4) works if Eq. (8.5) holds. Of course you can construct an infinite number of potentials of the form given by Eq. (8.1), but I discuss only the free particle, infinite square well, and simple harmonic oscillator potential. These are the separable potentials of physical interest.

8.1.1 Free Particle

In the case of a free particle having mass m, the eigenfunctions are

$$\psi_{\mathbf{p}}(\mathbf{r}) = \psi_{p_x}(x)\,\psi_{p_y}(y)\,\psi_{p_z}(z) = \frac{1}{(2\pi\hbar)^{3/2}} e^{ip_x x/\hbar} e^{ip_y y/\hbar} e^{ip_z z/\hbar}$$
$$= \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}, \tag{8.6}$$

with

$$E_p = \frac{p_x^2 + p_y^2 + p_z^2}{2m} = \frac{p^2}{2m}. \tag{8.7}$$

I have already discussed this solution in Chaps. 3 and 5.

8.1.2 Two- and Three-Dimensional Infinite Wells

For a particle having mass m moving in a two-dimensional, infinite height rectangular well potential located between $0 \le x \le a_x$; $0 \le y \le a_y$, the eigenfunctions are

$$\psi_{n_x,n_y}(x, y) = \sqrt{\frac{2}{a_x}\frac{2}{a_y}} \sin\left(\frac{n_x \pi x}{a_x}\right) \sin\left(\frac{n_y \pi y}{a_y}\right);$$
$$n_x, n_y = 1, 2, 3, \ldots, \tag{8.8}$$

with

$$E_{n_x,n_y} = \frac{\hbar^2 \pi^2}{2m}\left[\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2}\right]. \tag{8.9}$$

If a_x and a_y are incommensurate, there is no energy degeneracy. If $a_x = a_y$, there is clearly at *least* a two-fold degeneracy when $n_x \neq n_y$. However, there is more degeneracy than this, in general. The problem reduces to a well-known problem in number theory to find pairs of integers n_x and n_y for which $n_x^2 + n_y^2 = n$, where n is an integer.[1] The degeneracy grows with increasing n, but very slowly, approximately as $\log \sqrt{n}$. There may be some underlying symmetry associated with this extra deneneracy, but I have yet to find it.

For a particle having mass m moving in a three-dimensional infinite well box potential, the eigenfunctions are

$$\psi_{n_x,n_y}(x,y) = \sqrt{\frac{2}{a_x}\frac{2}{a_y}\frac{2}{a_z}} \sin\left(\frac{n_x \pi x}{a_x}\right) \sin\left(\frac{n_y \pi y}{a_y}\right) \sin\left(\frac{n_z \pi z}{a_z}\right);$$
$$n_x, n_y, n_z = 1, 2, 3, \ldots, \tag{8.10}$$

with

$$E_{n_x,n_y,n_z} = \frac{\hbar^2 \pi^2}{2m}\left[\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2}\right]. \tag{8.11}$$

If $a_x = a_y = a_z$ the degeneracy of the states increases roughly linearly with $n = \sqrt{n_x^2 + n_y^2 + n_z^2}$.

8.1.3 SHO in Two and Three Dimensions

It is a trivial matter to solve the SHO problem in two and three dimensions using rectangular coordinates. In two dimensions the Hamiltonian is

$$\hat{H} = \hat{H}_x + \hat{H}_y, \tag{8.12a}$$

$$\hat{H}_x = \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m \omega_x^2 \hat{x}^2, \tag{8.12b}$$

$$\hat{H}_y = \frac{\hat{p}_y^2}{2m} + \frac{1}{2} m \omega_y^2 \hat{y}^2. \tag{8.12c}$$

The eigenenergies are

$$E_{n_x,n_y} = \hbar\omega_x\left(n_x + \frac{1}{2}\right) + \hbar\omega_y\left(n_y + \frac{1}{2}\right); \quad n_x, n_y = 0, 1, 2, 3, \ldots \tag{8.13}$$

[1]This problem in number theory is related to the so-called Ramanujan or "taxi cab" numbers. The famous number theorist Srinivasa Ramanujan is said to have commented on a taxi-cab number, 1729, as a very interesting number, since it is the smallest number expressible as the sum of two cubes in two different ways, $1^3 + 12^3$ or $9^3 + 10^3$. Generalized Ramanujan numbers are different integral solutions $\{n_1, n_2\}$ to the equation $n_1^m + n_2^m = n$, for integer n and m.

and eigenfunctions are

$$\psi_{n_x,n_y}(x,y) = \psi_{n_x}(x)\,\psi_{n_y}(y)\,, \tag{8.14}$$

where $\psi_{n_x}(x)$ and $\psi_{n_y}(y)$ are eigenfunctions of $\hat{H}_x$ and $\hat{H}_y$, respectively, given by Eq. (7.46b). If ω_x and ω_y are incommensurable, there is no degeneracy. In the limit that $\omega_x = \omega_y = \omega$, I can write the energy as

$$E_n = \hbar\omega\,(n+1)\,, \tag{8.15}$$

with

$$n = n_x + n_y. \tag{8.16}$$

In this case there is an $(n+1)$-fold degeneracy.

Similarly, in three dimensions, the eigenenergies are

$$E_{n_x,n_y,n_z} = \hbar\omega_x\left(n_x + \frac{1}{2}\right) + \hbar\omega_y\left(n_y + \frac{1}{2}\right) + \hbar\omega_z\left(n_z + \frac{1}{2}\right) \tag{8.17}$$

$\left(n_x, n_y, n_z = 0, 1, 2, 3, \ldots\right)$ and eigenfunctions are

$$\psi_{n_x,n_y,n_z}(x,y,z) = \psi_{n_x}(x)\,\psi_{n_y}(y)\,\psi_{n_z}(z)\,. \tag{8.18}$$

In the limit that $\omega_x = \omega_y = \omega_z = \omega$,

$$E_n = \hbar\omega\left(n + \frac{3}{2}\right), \tag{8.19}$$

with

$$n = n_x + n_y + n_y. \tag{8.20}$$

In this case there is an $(n+1)\,(n+2)\,/2$-fold degeneracy.

8.2 General Hamiltonians in Two and Three Dimensions

If there is no symmetry in the problem and the Hamiltonian is not a sum of the form of Eq. (8.1), you are faced with solving the Schrödinger equation numerically, in general. However, if there is symmetry, you can identify operators that commute with the Hamiltonian. For example, with cylindrical symmetry, the z component of linear momentum and z component of angular momentum commute with the

Hamiltonian; in this limit, the eigenfunctions are products of $e^{ip_z z/\hbar}e^{im\phi}$ (m must be integral for the wave function to return to itself when $\phi \to \phi + 2\pi$) times some function of the radial (cylindrical) coordinate. There is always energy degeneracy in this problem for $m \neq 0$ since states having $\pm m$ must have the same energy since the potential is invariant under a rotation about the z axis. In the case of problems with spherical symmetry, the angular momentum is conserved and can be used to classify the solutions. I turn my attention to problems with spherical symmetry in the next two chapters.

8.3 Summary

I have taken a brief excursion to look at some simple problems in two and three dimensions. In problems lacking some global symmetries, it is possible to arrive at some systematic solution of the Schrödinger equation only for separable Hamiltonians.

8.4 Problems

1. Prove that the trial solution (8.4) is an eigenfunction of the Hamiltonian (8.3) if Eq. (8.5) holds.

2. Find the eigenfunctions and eigenenergies of an infinite, two-dimensional square well having equal sides L. That is

$$V(x,y) = 0 \qquad 0 \le x \le L,\ 0 \le y \le L$$

and is infinite otherwise. In general, there is at least a two-fold degeneracy of the energy levels, but, in certain cases, show that there can be no degeneracy or greater than two-fold degeneracy.

3. Prove that the energy degeneracy for the isotropic 2-D oscillator is $(n+1)$ and that for the isotropic 3-D oscillator is $(n+1)(n+2)/2$.

4. Prove that the parity of the eigenfunctions of both the isotropic 2-D oscillator and the isotropic 3-D oscillator is $(-1)^n$.