A Particle in an Isoceles Right Triangle

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The particle-in-a-box problem is treated in almost every introductory quantum chemistry text. When the box is a square (or a cube), the method of separation of variables is usually employed. Indeed, the simple problem of particle in a square is ideally suited for the introduction of the separation-of-variables technique, which can then be applied to the more complicated case of the hydrogen atom. However, when the particle is confined to an isoceles right triangle, i.e., half of a square, it will be seen that the wave function of this two-dimensional system is no longer the simple product of two functions each involving only one variable.

The coordinate system chosen for this problem is shown in the figure. The Schrödinger equation is of the form

$$(-h^2/8\mu\pi^2)[(\partial^2/\partial x^2) + (\partial^2/\partial y^2)]\psi = E\psi \qquad (1)$$

where μ is the mass of the particle. The boundary conditions for the present case are (1) ψ vanishes when $x = 0$ or $y = 0$ and (2) ψ vanishes when $x + y = a$. Solutions that satisfy condition (1), but not (2), are the well-known results for the particle-in-a-square problem:

$$\psi_{mn} = [(2/a)^{1/2} \sin(m\pi x/a)][(2/a)^{1/2} \sin(n\pi y/a)] \qquad (2)$$

$$E_{mn} = (h^2/8\mu a^2)(m^2 + n^2) \qquad m,n = 1, 2, 3, \ldots \qquad (3)$$

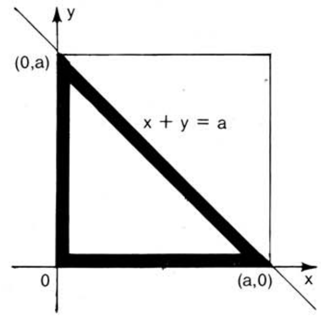
Since the expression for E_{mn} as given in eqn. (3) is symmetrical with respect to the exchange of m and n, i.e., $E_{mn} = E_{nm}$, ψ_{mn} and ψ_{nm} are degenerate wave functions.

In order to have solutions that also meet condition (2), we first linearly combine ψ_{mn} and ψ_{nm}:

$$\begin{aligned}\psi'_{mn} &= (2)^{-1/2}(\psi_{mn} + \psi_{nm}) \\ &= [(2)^{1/2}/a][\sin(m\pi x/a)\sin(n\pi y/a) \\ &\quad + \sin(n\pi x/a)\sin(m\pi y/a)]\end{aligned} \qquad (4)$$

$$\begin{aligned}\psi''_{mn} &= (2)^{-1/2}(\psi_{mn} - \psi_{nm}) \\ &= [(2)^{1/2}/a][\sin(m\pi x/a)\sin(n\pi y/a) \\ &\quad - \sin(n\pi x/a)\sin(m\pi y/a)]\end{aligned} \qquad (5)$$

When $m = n$, ψ'_{mn} is simply ψ_{mm} (aside from a numerical factor) and ψ''_{mm} vanishes; hence, neither ψ'_{mm} nor ψ''_{mm} is an acceptable solution. On the other hand, when $m = n \pm 1$, $n \pm 3, \ldots, \psi'_{mn}$ vanishes when $x + y = a$; also, when $m = n \pm 2, n \pm 4, \ldots, \psi''_{mn}$ vanishes under the same condition. Thus, ψ'_{mn} $(m = n \pm 1, n \pm 3, \ldots)$ and ψ''_{mn} $(m = n \pm 2, n \pm 4, \ldots)$ are the solutions to the present problem. It is noted that these wave functions are not products of two functions each involving only one variable. In addition, the energy expression now becomes



Coordinate system for the problem of particle in an isoceles right triangle.

$$E_{mn} = (h^2/8\mu a^2)(m^2 + n^2), \qquad m,n = 1, 2, 3, \ldots \text{ and } m \neq n \qquad (6)$$

Since only one wave function can be written for a set of quantum numbers (m,n), i.e., $\psi'_{mn} = \psi'_{nm}$ and $\psi''_{mn} = \psi''_{nm}$ (aside from a negative sign), the degeneracy in the particle-in-a-square problem, i.e., $E_{mn} = E_{nm}$ in eqn. (3), is now removed. This is expected as there is a reduction in symmetry from D_{4h} (square box) to C_{2v} (isoceles right triangular box). Still, some "unforeseen" degeneracies remain in the right-triangular case, for example, $E_{1,8} = E_{4,7}$. These degeneracies have been discussed in connection with the particle-in-a-square problem elsewhere.[1,2]

Finally, it is noted that the particle-in-an-equilateral-triangle problem has also been treated recently.[3]

[1] Shaw, G. B., *J. Phys. A*, **7**, 1357 (1974).
[2] Li, W.-K., *J. Am. Phys.*, **50**, 666 (1982).
[3] Krishnamurthy, H. R., Mani, H. S., and Verma, H. C., *J. Phys. A*, **15**, 2131 (1982).