AIP | Journal of Mathematical Physics

Solution of the Schrödinger equation for a particle in an equilateral triangle

Wai-Kee Li and S. M. Blinder

Citation: Journal of Mathematical Physics **26**, 2784 (1985); doi: 10.1063/1.526701
View online: http://dx.doi.org/10.1063/1.526701
View Table of Contents: http://scitation.aip.org/content/aip/journal/jmp/26/11?ver=pdfcov
Published by the AIP Publishing

Solution of the Schrödinger equation for a particle in an equilateral triangle

Wai-Kee Li
Department of Chemistry, Chinese University of Hong Kong, Shatin, N. T., Hong Kong
S. M. Blinder
Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109

(Received 25 April 1985; accepted for publication 12 June 1985)

The complete solution for the quantum-mechanical problem of a particle in an equilateral triangle is derived. By use of projection operators, eigenfunctions belonging explicitly to each of the irreducible representations of the symmetry group C_{3V} are constructed. The most natural definition of the quantum numbers p and q includes not only integers but also nonintegers of the class $\frac{1}{3}$ and $\frac{2}{3}$ modulo 1. Some relevant features relating to symmetry and degeneracy are also discussed.

I. INTRODUCTION

The two-dimensional Schrödinger equation for a particle confined within an equilateral triangle has been considered by several authors.[1–4] Mathews and Walker[1] derived a solution in the form of a double Fourier series after generating a periodic lattice by successive reflections and rotations of the triangle. Krishnamurthy *et al.*[2] applied an ingenious transformation of the solution for three fermions in a one-dimensional segment into that for a single particle in a triangle. Shaw[3] reduced the Schrödinger equation to a quasi-one-dimensional form involving a complex coordinate $z = x + iy$. However, he obtained only those eigenstates transforming as the A_1 and A_2 representations of the symmetry group C_{3V}. The corresponding problem in a classical context was solved by Lamé[4] a very long time ago.

The various solutions of the problem result in functional forms and energy expressions of rather different appearance. In common with the problem of the isosceles right triangle, recently solved by one of us,[5] the Schrödinger equation for the equilateral triangle is *not* soluble by separation of variables. Recently, analogous nonseparable solutions for tetrahedral boxes also have been obtained.[2,6]

II. METHOD OF SOLUTION

We seek solutions of the Schrödinger equation

$$-\left(\frac{\hbar^2}{2m}\right)\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]\Psi(x,y) = E\Psi(x,y), \qquad (1)$$

such that $\Psi(x,y) = 0$ on the three sides of an equilateral triangle of side a situated as shown in Fig. 1(a). It is convenient to introduce the altitude of the triangle, given by $A = (\sqrt{3}/2)a$. The three boundary conditions thus require that

$$\Psi(x,y) = 0, \quad \text{when} \begin{cases} y = 0, \\ y = \sqrt{3}x, \\ y = \sqrt{3}(a-x) = 2A - \sqrt{3}x. \end{cases} \qquad (2)$$

It will be expedient to introduce three auxiliary variables

$$u = (2\pi/A)y, \quad v = (2\pi/A)(-y/2 + \sqrt{3}x/2),$$
$$w = (2\pi/A)(-y/2 - \sqrt{3}x/2) + 2\pi. \qquad (3)$$

These are proportional to the perpendicular distances from an interior point to the three sides of the triangle, as shown in Fig. 1(b). The sum of these perpendiculars equals the altitude of the triangle and thus

$$u + v + w = 2\pi. \qquad (4)$$

The boundary conditions (2) now assume the more symmetrical form

$$\Psi = 0, \quad \text{when} \begin{cases} u = 0, & v = 2\pi - w, \\ v = 0, & w = 2\pi - u, \\ w = 0, & u = 2\pi - v. \end{cases} \qquad (5)$$

The equilateral triangle problem is invariant under the point group C_{3V}. Equivalently, the sides (or vertices) can be permuted according to the symmetric group S_3, isomorphic with C_{3V}. Let the variables u,v,w transform under S_3 as follows:

$$C_3\colon\ u \leftarrow v \leftarrow w \leftarrow u, \quad C_3^2\colon\ u \rightarrow v \rightarrow w \rightarrow u,$$
$$\sigma_1\colon\ u \leftrightarrow v, \quad \sigma_2\colon\ w \leftrightarrow u, \quad \sigma_3\colon\ v \leftrightarrow w. \qquad (6)$$

Thus the vector (u,v,w) generates the following 3×3 reducible representation of S_3 or C_{3V}:

$$E = \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}, \quad C_3 = \begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix},$$
$$C_3^2 = \begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}, \quad \sigma_1 = \begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}, \qquad (7)$$
$$\sigma_2 = \begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix}, \quad \sigma_3 = \begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix}.$$

Boundary conditions aside, the free-particle Schrödinger equation (1) admits solutions of the form $f(c_1x + c_2y)$, in which $f(z)$ is a harmonic function such as $\sin z$, $\cos z$, or $\exp(\pm iz)$. With the use of Eqs. (3), let this function be expressed in the form $f(pu - qv)$, in which p and q are constants.

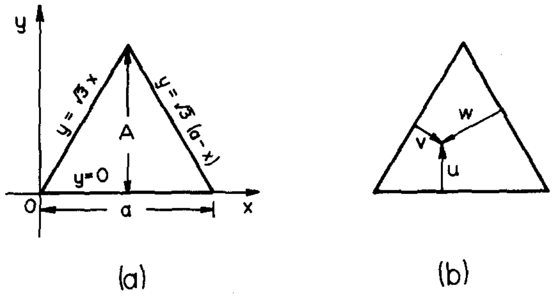

FIG. 1. (a) The coordinate system for an equilateral triangle showing boundary conditions. (b) The auxiliary variables u,v,w.

III. A_1 SOLUTIONS

We shall next construct C_{3V}-symmetry adapted functions by application of projection operators. Recall that C_{3V} admits of three irreducible representations: A_1 and A_2, which are nondegenerate, and E, which is doubly degenerate. The A_1 projection operator

$$\mathscr{P}(A_1) = E + C_3 + C_3^2 + \sigma_1 + \sigma_2 + \sigma_3, \tag{8}$$

applied to the "basis function" $f(pu - qv)$, with the use of (6), gives

$$\Psi_{p,q}(A_1) = f(pu - qv) + f(pv - qw) + f(pw - qu) + f(pv - qu) + f(pw - qv) + f(pu - qw). \tag{9}$$

It is readily shown that the boundary conditions (5) can be fulfilled only if $f = \sin$ and p,q are integers. We find further that

$$\Psi_{q,p} = -\Psi_{p,q},\quad \Psi_{-p,-q} = -\Psi_{p,q},\quad \Psi_{p+q,-p} = -\Psi_{p,q}. \tag{10}$$

Thus, without loss of generality, the quantum numbers p,q can be restricted such that $p > q \geqslant 0$, with p and q integral. The eigenfunctions (9) can be reduced to more compact trigonometric forms as follows:

$$\begin{aligned}\Psi_{p,q}(A_1) = {} & \cos[q\sqrt{3}\pi x/A]\sin[(2p+q)\pi y/A] \\ & - \cos[p\sqrt{3}\pi x/A]\sin[(2q+p)\pi y/A] \\ & - \cos[(p+q)\sqrt{3}\pi x/A]\sin[(p-q)\pi y/A], \\ & q = 0,1,2,\ldots,\quad p = q+1, q+2,\ldots .\end{aligned} \tag{11}$$

Specifically, for $q = 0$,

$$\Psi_{p,0}(A_1) = \sin(2p\pi y/A) - 2\sin(p\pi y/A) \times \cos(p\sqrt{3}\pi x/A),\quad p = 1,2,3\ldots . \tag{12}$$

Note that the above functions are not normalized. These agree with the specific cases listed by Shaw.[3] The energy eigenvalues corresponding to (11) and (12) are given by

$$E_{p,q} = (p^2 + pq + q^2)E_0,\quad E_0 \equiv h^2/2mA^2 = E_{1,0}. \tag{13}$$

IV. A_2 SOLUTIONS

For the A_2 representations, the projection operator

$$\mathscr{P}(A_2) = E + C_3 + C_3^2 - \sigma_1 - \sigma_2 - \sigma_3 \tag{14}$$

applied to $f(pu - qv)$ results in

$$\Psi_{p,q}(A_2) = f(pu - qv) + f(pv - qw) + f(pw - qu) - f(pv - qu) - f(pw - qv) - f(pu - qw). \tag{15}$$

These fulfill the boundary conditions with $f = \cos$ and, again, for integral p,q. In analogy with (10), we find for the A_2 functions,

$$\Psi_{q,p} = -\Psi_{p,q},\quad \Psi_{-p,-q} = \Psi_{p,q},\quad \Psi_{p+q,-q} = -\Psi_{p,q}. \tag{16}$$

The last relation shows that $\Psi_{p,q} = 0$ if $q = 0$. Otherwise the same spectrum as the A_1 functions is obtained, with $p > q > 0$, p and q integral. The A_2 eigenfunctions in trigonometric form analogous to (11) are given by

$$\begin{aligned}\Psi_{p,q}(A_2) = {} & \sin[q\sqrt{3}\pi x/A]\sin[(2p+q)\pi y/A] \\ & - \sin[p\sqrt{3}\pi x/A]\sin[(2q+p)\pi y/A] \\ & + \sin[(p+q)\sqrt{3}\pi x/A]\sin[(p-q)\pi y/A], \\ & q = 1,2,3,\ldots,\quad p = q+1, q+2,\ldots .\end{aligned} \tag{17}$$

The eigenvalues are again given by (13), except that $q = 0$ is missing. Remarkably, every A_2 eigenstate is degenerate with an A_1 eigenstate carrying the same quantum numbers. The only nondegenerate eigenstates are the A_1 with $q = 0$. A similar situation arises for a particle in a square, as discussed by Shaw,[3] in which there occur degenerate pairs of $A_1 + B_1$ species and again of $A_2 + B_2$ species.

V. E SOLUTIONS

Finally, for the E representation, we make use of the projection operator

$$\mathscr{P}(E) = E + \epsilon C_3 + \epsilon^* C_3^2 - \sigma_1\mathscr{C} - \epsilon\sigma_2\mathscr{C} - \epsilon^*\sigma_3\mathscr{C}, \tag{18}$$

where $\epsilon = \exp(2\pi i/3)$ and $\mathscr{C}$ represents the operation of complex conjugation. Applying (18) to $f(pu - qv)$ we obtain

$$\begin{aligned}\Psi_{p,q}(E) = {} & f(pu - qv) + \epsilon f(pv - qw) \\ & + \epsilon^* f(pw - qu) - f^*(pv - qu) \\ & - \epsilon f^*(pw - qv) - \epsilon^* f^*(pu - qw).\end{aligned} \tag{19}$$

The boundary conditions are satisfied with the function $f(z) = \exp(+iz)$, but now with $p,q = n + \frac{1}{3}$ (n = integer). The complex conjugate of (19) gives the partner in this degenerate representation. One can alternatively apply (18) with $\epsilon = \exp(-2\pi i/3)$. This generates a second class of E eigenfunctions (19) with $p,q = n + \frac{2}{3}$. The following relationships among the E functions can be demonstrated:

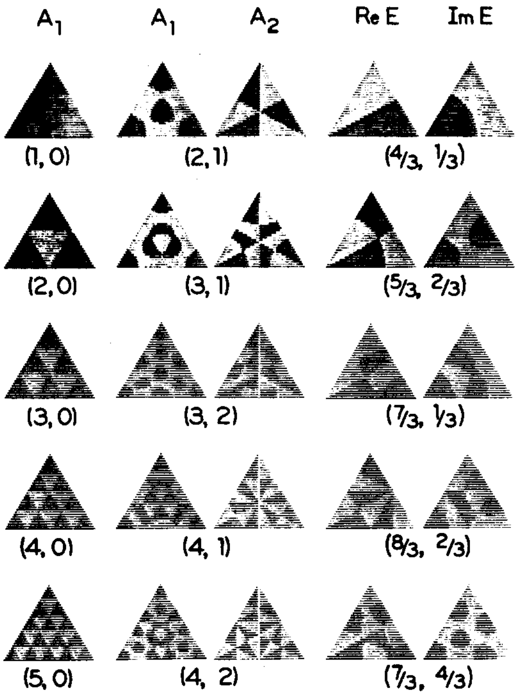

FIG. 2. The graphical representation of some lower eigenstates (p,q) of each symmetry type. For visual simplicity, only the sign (+ or −) of the wave function is plotted.

$$\begin{aligned}\Psi_{q,p} &= -\Psi_{p,q},\\ \Psi_{-p,-q} &= \Psi^*_{p+1/3,q+1/3},\\ \Psi_{p+q,-p} &= -\Psi^*_{p+1/3,q+1/3}.\end{aligned} \tag{20}$$

Thus, E states can be labeled by the quantum numbers $q=\frac{1}{3},\frac{2}{3},\frac{4}{3},\frac{5}{3},\ldots$, $p=q+1,q+2,\ldots$. The real and imaginary parts of $\Psi_{p,q}(E)$ turn out to have the same forms as (17) and (11), respectively, but with p,q now equal to $\frac{1}{3}$ or $\frac{2}{3}$ modulo 1, viz.,

$$\begin{aligned}\mathrm{Re}\,\Psi_{p,q}(E) &= \Psi_{p,q}(A_2),\\ \mathrm{Im}\,\Psi_{p,q}(E) &= \Psi_{p,q}(A_1),\\ q=\tfrac{1}{3},\tfrac{2}{3},\tfrac{4}{3},\tfrac{5}{3},\ldots,&\quad p=q+1,q+2,\ldots.\end{aligned} \tag{21}$$

VI. SUMMARY

The Schrödinger equation (1) subject to the boundary conditions (2) has solutions $\Psi_{p,q}$. The A_1 eigenfunctions are given by Eq. (9) or Eq. (11) [Eq. (12) if $q=0$], the A_2 eigenfunctions by Eq. (15) or Eq. (17), and the E eigenfunctions by Eq. (19) or Eq. (21). Figure 2 represents some of the lower-energy eigenfunctions of each symmetry species. For visual simplicity, only the sign of the wave function (+ or −) is plotted. The energy eigenvalues are given by the formula

$$E_{p,q}=(p^2+pq+q^2)E_0,$$

$$q=\begin{cases}0,1,2,\ldots, & \text{for } A_1,\\ 1,2,3,\ldots, & \text{for } A_2,\\ \frac{1}{3},\frac{2}{3},\frac{4}{3},\frac{5}{3},\ldots, & \text{for } E,\end{cases}$$

$$p=q+1,q+2,\ldots.$$

As discussed in Refs. 3 and 7, systems of high symmetry often exhibit "accidental" degeneracies beyond those implied by the purely geometrical symmetry of the Hamiltonian. Thus, in the equilateral triangle problem, $E=49$ (in units of E_0) represents a threefold-degenerate level compounded of an A_1 state with a A_1-A_2 pair, corresponding to the $(p,q)=(7,0)$ and (5,3). This is the first of an infinite number of such combinations. The first fourfold degeneracy from two coinciding A_1-A_2 pairs occurs for $E=91$, with $(p,q)=(6,5)$ and (9,1). We eventually encounter a sixfold degeneracy at $E=1519$ with states (23,22), (33,10), (35,7) and an eightfold degeneracy at $E=1729$ with states (25,23), (32,15), (37,8), (40,3). Degeneracies also arise from coincident E levels. Thus $E=30\frac{1}{3}$ is fourfold degenerate with states $(\frac{11}{3},\frac{8}{3})$ and $(\frac{16}{3},\frac{1}{3})$; $E=212\frac{1}{3}$ is sixfold degenerate with states $(\frac{31}{3},\frac{19}{3})$, $(\frac{35}{3},\frac{14}{3})$ and $(\frac{41}{3},\frac{5}{3})$. Such nongeometrical degeneracies can often be enumerated by applying results from number theory. For example, the number of integer combinations (m,n) such that m^2+mn+n^2 equals a particular integer is calculable.[8]

An amusing correspondence can be drawn between equilateral triangle eigenstates and families of leptons and quarks. The doubly degenerate levels with the quantum numbers $n+\frac{1}{3}$ and $n+\frac{2}{3}$ are quite suggestive of pairs of quarks (right and left handed) with charge $+\frac{1}{3}$ and $-\frac{2}{3}$, respectively. Similarly, the degenerate A_1,A_2 states might correspond to pairs of (right and left) leptons such as electrons or muons. Finally, the nondegenerate A_1's with $q=0$ suggest left-handed neutrinos (the right-handed partners being nonexistent).

[1] J. Mathews and R. L. Walker, *Mathematical Methods for Physicists* (Benjamin, New York, 1970), 2nd ed. pp. 237ff.
[2] H. R. Krishnamurthy, H. S. Mani, and H. C. Verma, J. Phys. A **15**, 2131 (1982). See also J. W. Turner, J. Phys. A **17**, 2791 (1984).
[3] G. B. Shaw, J. Phys. A **7**, 1357 (1974).
[4] M. G. Lamé, *Leçons sur la Théorie Mathèmatique de l'Elasticité des Corps Solides* (Bachelier, Paris, 1852), §57.
[5] W-K. Li, J. Chem. Educ. **61**, 1034 (1984).
[6] J. W. Turner, J. Phys. A **17**, 2791 (1984).
[7] W-K. Li, Am. J. Phys. **50**, 666 (1982).
[8] See, for example, E. D. Bolker, *Elementary Number Theory* (Benjamin, New York, 1970), p. 121.