Particle in an Equilateral Triangle: Exact Solution of a Nonseparable Problem

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In a recent note in *this Journal* (*1*), we discussed the quantum-mechanical problem of a particle in an isosceles right triangle. We showed that the eigenfunctions for this two-dimensional system are *not* separable functions of two variables even though the problem is exactly solvable. The particle in an equilateral triangle also has nonseparable exact solutions but proves to be considerably more complex. The Schrödinger equation has been solved by at least four different approaches (*2–6*). However, the results are so dissimilar that, at first reading, the eigenfunctions and even the energy expressions appear quite unrelated. Moreover, in two of the formulations, multiple sets of quantum numbers are required to specify a single state.

A particle confined within an equilateral triangle of side a is described by the Schrödinger equation

$$-(\hbar^2/2m)\,(\partial^2/\partial x^2 + \partial^2/\partial y^2)\,\psi(x,y) = E\psi(x,y) \tag{1}$$

such that $\psi(x,y)$ vanishes on the perimeter of the triangle. With the coordinate system as defined in Figure 1, the boundary conditions take the form $\psi(x,y) = 0$ for $y = 0$, $y = \sqrt{3}x$ or $y = \sqrt{3}(a - x)$.

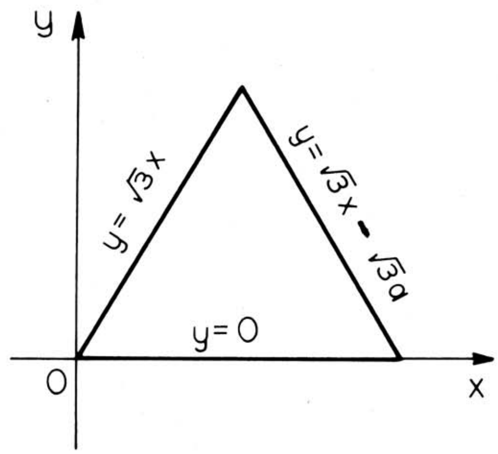

Figure 1. Coordinate system for equilateral triangle. Equations of the three sides specify boundary conditions.

We consider first the elegant solution of Mathews and Walker (*3*) (hereafter abbreviated MW). They constructed a lattice of equilateral triangles filling the xy-plane by repeated reflection of the original triangle through each of its sides (see Fig. 2). Consistent with the above boundary conditions, one can require that the wavefunction $\psi(x,y)$, whose domain is now the entire xy-plane, change sign with each reflection. Thus, as shown in Figure 2, reflecting OAB through side B gives ABD. The antisymmetry of the wavefunction is indicated by the disposition of + and − signs. Repeating the reflections in a horizontal direction eventually produces triangle CEF, in which the wavefunction is identical to that in the original triangle OAB. This implies the following periodicity in the wavefunction:

$$\psi(x + 3a,y) = \psi(x,y) \tag{2}$$

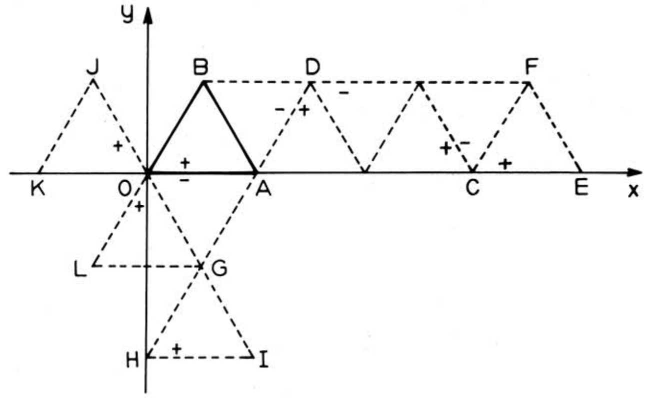

Figure 2. Original triangle OAB and part of triangular lattice generated by reflections and rotations.

An analogous series of vertical reflections shows the wavefunction to be identical in triangles OAB and HIG. Since the altitude of an equilateral triangle equals $(\sqrt{3}/2)a$, this implies the periodicity

$$\psi(x,y + \sqrt{3}a) = \psi(x,y) \tag{3}$$

Given its periodic structure, the wavefunction can be expanded in a double Fourier series as follows:

$$\psi(x,y) = \sum_{j=0}^{\infty}\sum_{k=0}^{\infty} a_{j,k}e^{2\pi ijx/3a}e^{2\pi iky/\sqrt{3}a} \tag{4}$$

Substituting $\psi(x,y)$ into eq 1 gives an expression for the energy eigenvalues:

$$E_{j,k} = (h^2/2ma^2)[(j^2/9) + (k^2/3)] \tag{5}$$

For each solution of the Schrödinger equation, the expansion (eq 4) contains only terms with indices j,k consistent with a single value of $E_{j,k}$ according to eq 5.

The symmetry properties of the system represented in Figure 2 imply further interrelationships among the coefficients $a_{j,k}$. For example, the signs in triangles OAB and OAG imply that $\psi(x,-y) = -\psi(x,y)$, so that

$$a_{j,k} = -a_{j,-k} \tag{6}$$

Further, when OAB is rotated by 120°, turning it into OJK, the wavefunction is unchanged, so that $\psi(-x/2 + \sqrt{3}y/2, -\sqrt{3}x/2 - y/2) = \psi(x,y)$. With use of eq 4, this implies

$$a_{j,k} = a_{j',k'} \quad (7)$$

when $j' = -(j/2) - (3k/2)$ and $k' = (j/2) - (k/2)$. A second rotation by 120°, into OGL, shows that $\psi(-x/2 - \sqrt{3}y/2, \sqrt{3}x/2 - y/2) = \psi(x,y)$, so that

$$a_{j,k} = a_{j'',k''} \quad (8)$$

when $j'' = -(j/2) + (3k/2)$ and $k'' = -(j/2) - (k/2)$. These symmetry conditions enable us to write down explicit forms for the wavefunctions. Thus the ground state corresponds to the (j,k) combinations (3,1), (3,−1), (−3,1), (−3,−1), (0,−2), (0,2). The ground state energy is given by

$$E_0 = 2h^2/3ma^2 \quad (9)$$

while relations 6–8 enable us to construct the corresponding eigenfunction:

$$\psi_0 = [3,1] - [3,-1] + [-3,1] - [-3,-1] + [0,-2] - [0,2] \quad (10)$$

in terms of the notation

$$[j,k] \equiv \exp(2\pi ijx/3a)\exp(2\pi iky/\sqrt{3}a) \quad (11)$$

The energies and wavefunctions of the first seven levels are presented in the table, with the MW functions given in one column. It can be readily checked that these functions do indeed obey the requisite boundary conditions. Note that six sets of indices are required to construct the MW eigenfunction for each state. For the doubly degenerate levels (more on these later), one state is transformed into the other by reversing the signs of each j and k. For the nondegenerate levels, sign reversal merely results in the negative of the wavefunction.

The structure of the MW functions, each consisting of three positive and three negative terms, is suggestive of a 3 × 3 determinant. Indeed, by approaching the problem from an entirely different direction, Krishnamurthy et al. (4) (KMV) arrived at solutions of the following form:

$$\psi_{l,m} = \begin{vmatrix} 1 & 1 & 1 \\ e^{2\pi ilx/3a}e^{2\pi ily/\sqrt{3}a} & e^{2\pi ilx/3a}e^{-2\pi ily/\sqrt{3}a} & e^{-4\pi ilx/3a} \\ e^{2\pi imx/3a}e^{2\pi imy/\sqrt{3}a} & e^{2\pi imx/3a}e^{-2\pi imy/\sqrt{3}a} & e^{-4\pi imx/3a} \end{vmatrix} \quad (12)$$

KMV obtained this result by an ingenious mapping of the solution of a one-dimensional, three-fermion problem into that for a single particle confined to an equilateral triangle. The KMV quantum numbers l,m are related to the MW indices j,k as follows:

$$l = (j + k)/2 \quad (13)$$

$$m = (j - k)/2 \quad (14)$$

In contrast to the MW functions, which require six sets of indices (j,k), the KMV functions can be defined by six alternative sets of quantum numbers (l,m). The ground state, for example, corresponds to (2,1), (1,2), (−1,−2), (−2,−1), (−1,1), or (1,−1). Each of the $\psi_{l,m}$ thus defined is then equal to either ψ_0 or $-\psi_0$, as given in eq 10. The alternative KMV quantum numbers are related, using eqs 6–8, 13, and 14, as follows:

$$\psi_{l,m} = -\psi_{m,l} \quad (15)$$

$$\psi_{l,m} = \psi_{m-l,-l} \quad (16)$$

$$\psi_{l,m} = \psi_{-m,l-m} \quad (17)$$

In terms of the KMV quantum numbers, the energy levels are given by

$$E_{l,m} = (2h^2/9ma^2)(l^2 - lm + m^2) = (l^2 - lm + m^2)E_0/3 \quad (18)$$

KMV eigenfunctions for the first seven levels are also listed in the table.

KMV point out that for $l + m = 3n$ (where n is an integer), the functions $\psi_{l,m} - \psi^*_{l,m}$ and $\psi_{l,m} + \psi^*_{l,m}$ transform, respectively, as the A_1 and A_2 representations of the symmetry group C_{3v}. For $l + m = 3n + 1$ or $3n + 2$, the pair $\psi_{l,m}$ and $\psi^*_{l,m}$ transform as the E representation.

We have given an alternative solution of the equilateral triangle problem based on its C_{3v} symmetry properties (5). We first define the auxiliary variables:

$$u \equiv (2\pi/A)y \quad (19)$$

$$v \equiv (2\pi/A)(-y/2 + \sqrt{3}x/2) \quad (20)$$

$$w \equiv (2\pi/A)(-y/2 - \sqrt{3}x/2) + 2\pi \quad (21)$$

such that

$$u + v + w = 2\pi \quad (22)$$

in which A represents the altitude of the triangle. The wavefunction vanishes, in accord with the boundary conditions, when $u = 0$, $v = 0$, or $w = 0$. The C_{3v} symmetry group of the triangle is isomorphous with the symmetric group S_3 representing the permutations among the variables u, v, w. Apart from boundary conditions, the free-particle Schrödinger equation (eq 1) admits harmonic solutions of the form $f(c_1x + c_2y)$ or, by virtue of eqs 19–22, $f(pu - qv)$, in which p and q are constants. We construct C_{3v}-symmetry adapted functions belonging to the irreducible representations A_1, A_2, and E, respectively, by applying the following projection operators to $f(pu - qv)$:

$$\mathcal{P}(A_1) = E + C_3 + C_3^2 + \sigma_1 + \sigma_2 + \sigma_3 \quad (23)$$

$$\mathcal{P}(A_2) = E + C_3 + C_3^2 - \sigma_1 - \sigma_2 - \sigma_3 \quad (24)$$

$$\mathcal{P}(E) = E + \epsilon C_3 + \epsilon^* C_3^2 - \sigma_1\mathcal{C} - \epsilon\sigma_2\mathcal{C} - \epsilon^*\sigma_3\mathcal{C} \quad (25)$$

$$\epsilon = \exp(+2\pi i/3) \quad (26)$$

Here $\mathcal{C}$ represents the operation of taking the complex conjugate. To fulfill the boundary conditions, f must represent the function sin, cos, and e^{+i}, respectively, for A_1, A_2, and E eigenfunctions. The explicit forms are as follows:

$$\psi_{pq}^{A_1} = \sin(pu - qv) + \sin(pv - qw) + \sin(pw - qu) + \sin(pv - qu) + \sin(pw - qv) + \sin(pu - qw) \quad (27)$$

where $q = 0, 1, 2, \ldots$ and $p = q + 1, q + 2, \ldots$.

$$\psi_{pq}^{A_2} = \cos(pu - qv) + \cos(pv - qw) + \cos(pw - qu) - \cos(pv - qu) - \cos(pw - qv) - \cos(pu - qw) \quad (28)$$

where $q = 1, 2, 3, \ldots$ and $p = q + 1, q + 2, \ldots$.

$$\psi_{pq}^{E} = \exp[i(pu - qv)] + \epsilon\exp[i(pv - qw)] + \epsilon^*\exp[i(pw - qu)] - \exp[-i(pv - qu)] - \epsilon\exp[-i(pw - qv)] - \epsilon^*\exp[-i(pu - qw)] \quad (29)$$

where, for $\epsilon = \exp(+2\pi i/3)$, $q = 1/3, 4/3, 7/3, \ldots$ and $p = q + 1, q + 2, \ldots$, while, for $\epsilon = \exp(-2\pi i/3)$, $q = 2/3, 5/3, 8/3, \ldots$ and $p = q + 1, q + 2, \ldots$.

The energy eigenvalues in the present scheme are given by yet another formula:

$$E_{pq} = (p^2 + pq + q^2)E_0 \quad (30)$$

where $E_0 = 2h^2/3ma^2$, $q = 0, 1/3, 2/3, 1, \ldots$ and $p = q + 1, q + 2, \ldots$. The ground state energy E_0 corresponds to E_{10}. More generally, E_{p0}, with $p = 1, 2, \ldots$, represents a nondegenerate A_1 level. E_{pq}, with p and q positive integers, represents a pair of degenerate A_1 and A_2 states. E_{pq}, with p and q nonintegers, which we can call "quark" quantum numbers, represents a twofold-degenerate E level.

In terms of p and q, a representative set of KMV quantum numbers is given by

$$l = 2p + q \quad (31)$$

$$m = p - q \quad (32)$$

Energies and Wavefunctions for First Seven Levels of Equilateral Triangle

(p, q) [a]	Energy [b]	Symmetry	$\psi^{MW} = \sum_j \sum_k a_{j,k}[j,k]$ [c]	(l,m) of $\psi^{KMV}_{l,m}$ [d]
(1, 0)	1	A_1	[3,1] − [3,−1] + [−3,1] − [−3,−1] + [0,−2] − [0,2]	(2,1) or (1,2) or (−1,−2) or (−2,−1) or (−1,1) or (1,−1)
(4/3, 1/3)	2.33	E	[5,1] − [5,−1] + [−4,2] − [−4,−2] + [−1,−3] − [−1,3];	(3,2) or (2,3) or (−1,−3) or (−3,−1) or (−2,1) or (1,−2);
			[−5,−1] − [−5,1] + [4,−2] − [4,2] + [1,3] − [1,−3]	(−3,−2) or (−2,−3) or (1,3) or (3,1) or (2,−1) or (−1,2)
(2, 0)	4	A_1	[6,2] − [6,−2] + [−6,2] − [−6,−2] + [0,−4] − [0,4]	(4,2) or (2,4) or (−2,−4) or (−4,−2) or (−2,2) or (2,−2)
(5/3, 2/3)	4.33	E	[2,4] − [2,−4] + [5,−3] − [5,3] + [−7,−1] − [−7,1];	(3,−1) or (−1,3) or (1,4) or (4,1) or (−4,−3) or (−3,−4);
			[−2,−4] − [−2,4] + [−5,3] − [5,−3] + [7,1] − [7,−1]	(−3,1) or (1,−3) or (−1,−4) or (−4,−1) or (4,3) or (3,4)
(7/3, 1/3)	6.33	E	[1,5] − [1,−5] + [7,−3] − [7,3] + [−8,−2] − [−8,2];	(3,−2) or (−2,3) or (2,5) or (5,2) or (−5,−3) or (−3,−5);
			[−1,−5] − [−1,5] + [−7,3] − [−7,−3] + [8,2] − [8,−2]	(−3,2) or (2,−3) or (−2,−5) or (−5,−2) or (5,3) or (3,5)
(2, 1)	7	A_1, A_2	[3,5] − [3,−5] + [6,−4] − [6,4] + [−9,−1] − [−9,1];	(4,−1) or (−1,4) or (1,5) or (5,1) or (−5,−4) or (−4,−5);
			[−3,−5] − [−3,5] + [−6,4] − [−6,−4] + [9,1] − [9,−1]	(−4,1) or (1,−4) or (−1,−5) or (−5,−1) or (5,4) or (4,5)
(3, 0)	9	A_1	[0,6] − [0,−6] + [9,−3] − [9,3] + [−9,3] − [−9,−3]	(3,−3) or (−3,3) or (3,6) or (6,3) or (−3,−6) or (−6,−3)

[a] See eq 30.
[b] Units of E_0.
[c] See eq 11.
[d] See eq 12.

The A_1 and A_2 functions can be reduced to more compact trigonometric forms as follows:

$$\psi^{A_1}_{pq} = \cos[q\sqrt{3}\pi x/A]\sin[(2p+q)\pi y/A] - \cos[p\sqrt{3}\pi x/A]\sin[(2q+p)\pi y/A] - \cos[(p+q)\sqrt{3}\pi x/A]\sin[(p-q)\pi y/A] \quad (33)$$

$$\psi^{A_1}_{po} = \sin(2p\pi y/A) - 2\sin(p\pi y/A)\cos(p\sqrt{3}\pi x/A) \quad (34)$$

$$\psi^{A_2}_{pq} = \sin[q\sqrt{3}\pi x/A]\sin[(2p+q)\pi y/A] - \sin[p\sqrt{3}\pi x/A]\sin[(2q+p)\pi y/A] + \sin[(p+q)\sqrt{3}\pi x/A]\sin[(p-q)\pi y/A] \quad (35)$$

The E eigenfunctions can analogously be reduced. From eq 29 we find that Re ψ^E_{pq} and Im ψ^E_{pq} are given, respectively, by eqs 35 and 33, but with quantum numbers p and q now having "quark" values.

Shaw (*6*) also solved the triangle problem by reformulation to a quasi one-dimensional equation involving the complex variable $x + iy$. He obtained the A_1 and A_2 solutions given in eqs 33–35 but appears to have overlooked the E eigenfunctions.

In Figure 3, we sketch the nodal structure of the first seven triangle levels, corresponding to the functions listed in the table.

It is clear from Figure 3 that all the A_2 functions and one from each pair of E functions possess a node bisecting the equilateral triangle into two 30–60–90 triangles. Thus, a particle in a 30–60–90 triangle has eigenstates given by eqs 30 and 35, with the allowed quantum numbers $q = 1/3, 2/3, 1, \ldots$ and $p = q + 1, q + 2, \ldots$.

As discussed in refs *6* and *7*, systems of high symmetry often exhibit "accidental" degeneracies beyond those implied by dimensionalities of irreducible representations. In the present case, for example, the first threefold degenerate level ($A_1 + A_1 + A_2$) occurs for $E = 49E_0$ with the (p, q) combinations (7, 0) and (5, 3). The first fourfold degenerate level ($E + E$) occurs for $E = (91/3)E_0$, with $(p, q) = (11/3, 8/3)$ and (16/3, 1/3). Such nongeometrical degeneracies can often be enumerated by applying results from number theory. For

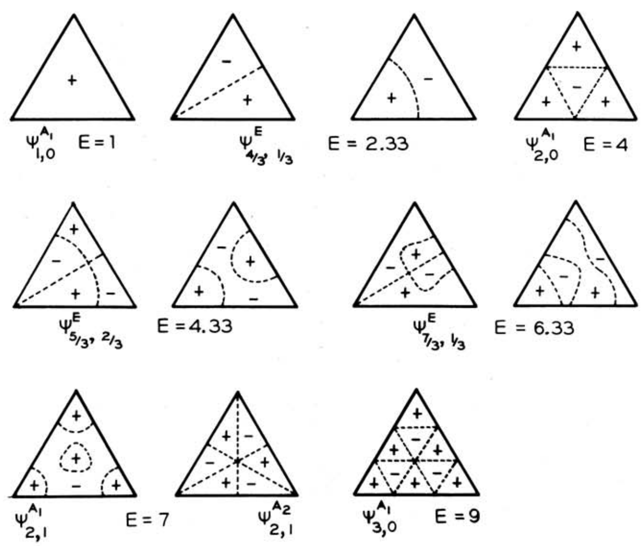

Figure 3. Graphical representation of eigenstates listed in the table. The nodal structure of the first seven levels is shown. Energies are expressed in units of E_0. The quantum numbers given are the (p, q) set.

example, the number of integer combinations (m, n) such that $m^2 + mn + n^2$ equals a particular integer is calculable (*8*).

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