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LETTER TO THE EDITOR

A class of exact solutions for anharmonically coupled oscillators

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Abstract. We study the solutions of the two-dimensional Schrödinger equation for anharmonically coupled oscillators. We obtain a finite set of exact solutions of the form $\psi(x, y) = \text{polynomial}\,(x, y)\exp(\text{polynomial}\,(x, y))$ provided that certain constraints on the potential parameters are satisfied.

The anharmonically coupled oscillator (ACO) models are used in studies concerned with approximate methods of solving the multidimensional Schrödinger equation. The first detailed study of the properties of the perturbation series for the energy of the ACO model with the potential $V(x, y) = \frac{1}{2}(\lambda_1 x^2 + \lambda_2 y^2) + \eta(xy)^2 + \xi_1 x^4 + \xi_2 y^4$ was performed by Bender and Wu (1973a, b). The numerical analysis of the same model with $\xi_i = 0$ is due to Caswell and Danos (1970). They proved the accuracy of the Born–Oppenheimer method in the separation of two coupled molecular vibrations. The models with coupling terms xy^2 (Hamiltonian of Barbanis (1966)) and $x(y^2 + \nu x^2)$ (Hamiltonian of Hénon and Heiles (1964)) were considered to establish the accuracy of the self-consistent field (Bowman 1978, Cohen *et al* 1979, Tobin and Bowman 1980, Christoffel and Bowman 1982) and adiabatic Born–Oppenheimer method (Zhi-Ding *et al* 1982). These models were also intensively used to study dynamics of the ACO system with semiclassical methods (Eastes and Marcus 1974, Noid and Marcus 1975, 1977, Noid *et al* 1979, 1980, Sorbie 1976, Sorbie and Handy 1977, Weisman and Jortner 1981a, b, 1982a, b).

The exact solutions of the Schrödinger equation for ACO models could serve as a useful device for the testing of practically oriented approximations, but till now such solutions have not been presented.

Recently, only for some anharmonic oscillators such solutions were found of the form $\psi(x) = P(x)\exp(R(x))$, where $P(x)$ and $R(x)$ are polynomials (Singh *et al* 1978, 1979, Flessas and Das 1980, Magyari 1981, Znojil 1981, 1982).

In this letter we propose the ACO models which have exact solutions of the analogous form

$$\psi(x, y) = P(x, y)\exp(R(x, y))$$

where $P(x, y)$ and $R(x, y)$ are polynomials of two variables. We also discuss some interesting properties of these solutions.

We shall be interested in solutions of the Schrödinger equation

$$(H(x, y) - E)\psi(x, y) = 0 \tag{1}$$

with the Hamiltonian

$$2H(x, y) = -(\partial^2/\partial x^2 + \partial^2/\partial y^2) + \lambda_1 x^2 + \lambda_2 y^2 + 2\eta\nu(xy)^2 + \eta^2(xy)^2(x^2+y^2). \tag{2}$$

This Hamiltonian is similar to that considered by Caswell and Danos (1970) if $\nu \gg \eta$, but is more realistic owing to the inclusion of the higher-order coupling term proportional to η^2. For $\eta < 0$ a potential with this term can have two or four minima. The potential with such properties has been used to describe pseudorotation in cyclic molecules (Carreira 1979).

Let us look for the solutions of equation (1) of the form

$$\psi(x, y) = P(x, y) \exp[-\tfrac{1}{2}(\omega_1 x^2 + \omega_2 y^2 + \eta x^2 y^2)] \tag{3}$$

where

$$P(x, y) = \sum_{n_1, n_2} a_{n_1, n_2} x^{2n_1+p_1} y^{2n_2+p_2},$$

$p_i = 0(1)$ for states of even (odd) parity with respect to x or y. We prove that $P(x, y)$ is a polynomial of the x and y variables if certain constraints on the parameters ω_i, λ_i and η are satisfied.

Substituting equation (3) into (1) we obtain difference equations for the unknown coefficients a_{n_1,n_2} which for $\nu = \omega_1 + \omega_2$ take the simple form

$$a_{n_1-1,n_2}B_1(n_2) + a_{n_1,n_2-1}B_2(n_1) + a_{n_1+1,n_2}C_1(n_1) + a_{n_1,n_2+1}C_2(n_2) = A_{n_1,n_2}a_{n_1,n_2} \tag{4}$$

where

$$B_i(n_j) = \eta[\gamma_i - (4n_j + 2p_j + 1)], \qquad i \neq j = 1, 2, \tag{5a}$$

$$C_i(n_i) = (2n_i + p_i + 2)(2n_i + p_i + 1), \tag{5b}$$

$$A_{n_1,n_2} = (4n_1 + 2p_1 + 1)\omega_1 + (4n_2 + 2p_2 + 1)\omega_2 - 2E, \tag{5c}$$

$$\gamma_i = (\omega_i^2 - \lambda_i)/\eta.$$

The $P(x, y)$ is a polynomial of N_1th degree with respect to x and N_2'th degree with respect to y if there exist such N_2 and N_1' that $a_{N_1,N_2} \neq 0$ and $a_{N_1',N_2'} \neq 0$ and $a_{n_1,n_2} = 0$ for every $n_1 > N_1$ and $n_2 > N_2'$.

Let us choose the index N_2 for which $a_{N_1,N_2} \neq 0$. In reality only one such N_2 exists, for if there is another $\tilde{N}_2 \neq N_2$, then taking in equation (4) $(n_1, n_2) = (N_1+1, N_2)$ we would obtain the condition

$$a_{N_1,N_2}B_1(N_2) = 0$$

which means

$$B_1(N_2) = 0, \tag{6a}$$

and taking $(n_1, n_2) = (N_1+1, \tilde{N}_2)$ we would obtain

$$a_{N_1,\tilde{N}_2}B_1(\tilde{N}_2) = 0$$

implying

$$B_1(\tilde{N}_2) = 0. \tag{6b}$$

It is clear now that equations $(6a, b)$ can be both fulfilled if and only if $N_2 = \tilde{N}_2$, so we draw the conclusion that only one N_2 exists. From this fact we can easily deduce that non-zero coefficients with the maximum n_1 for a given $N_2 \pm k$ are

$$a_{N_1-k,N_2+k} \qquad \text{for } k=0,1,\ldots,N_2'-N_2,$$
$$a_{N_1-k,N_2-k} \qquad \text{for } k=0,1,\ldots,N_2.$$

In a similar way we prove that there exists only one index N_1' for which $a_{N_1',N_2'}B_2(N_1')=0$ and $B_2(N_1')=0$. The non-zero coefficients with the maximum n_2 for a given $N_1' \pm k$ are

$$a_{N_1'+k,N_2'-k} \qquad \text{for } k=0,1,\ldots,N_1-N_1',$$
$$a_{N_1'-k,N_2'-k} \qquad \text{for } k=0,1,\ldots,N_1'.$$

To make our considerations easily understandable we present in figure 1 the graph of the polynomial P in which open (full) circles denote zero (non-zero) a_{n_1,n_2} coefficients. The crossed circles stand for the critical coefficients a_{N_1,N_2} and $a_{N_1'N_2'}$ which fulfil the equations (see equations (4))

$$\begin{aligned} A_{N_1,N_2}a_{N_1,N_2}&=0, \qquad & A_{N_1,N_2}&=0, \\ A_{N_1',N_2'}a_{N_1',N_2'}&=0, \qquad & A_{N_1',N_2'}&=0. \end{aligned} \tag{7}$$

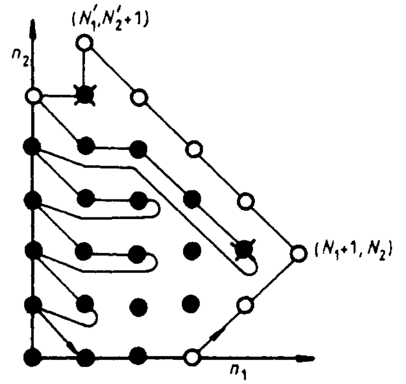

Figure 1. The graph of the polynomial $P(x, y)$ and the path generating all the points of $a_{n,m} \neq 0$.

Relations (7) impose the constraints on the energy E and frequencies ω_1, ω_2, thus providing for the existence of the solutions of equations (4). Let us note that the equations

$$B_1(N_2)=B_2(N_1')=0$$

relate the parameters λ_i and η and the frequencies ω_i through the two conditions

$$\gamma_1=4N_2+2p_2+1, \qquad \gamma_2=4N_1'+2p_1+1. \tag{8}$$

Thus, only one degree of freedom of these parameters remains.

Equations (4) can now be easily solved with the use of the topology of the graph P in the following way. Let us determine a path in the graph such that starting from $a_{N_1-N_2+1,0}$ and moving along the path we generate subsequently, from recurrence relations (4), all the points of $a_{n'm} \neq 0$. Instead of describing verbally an algorithm defining this path we present it in figure 1, from which we can clearly see that it can always be found. All points lying on the path are uniquely determined by $a_{N_1-N_2,0}$. However, f points ($f = N_1 + N_2 - 1$ for $N_i > 2$) exist which do not lie on the path, which means that in general f equations from equations (4) will not be fulfilled.

The proper choice of λ_i, η parameters can only guarantee that one of the f equations will be fulfilled since there is only one degree of freedom in the parametric space. So, the necessary but not sufficient condition for the existence of non-trivial solutions of equations (4) is $f \leqslant 1$. This condition means that only the polynomials for which $N_1 \leqslant 2$ and $N_2 \leqslant 2$ can exist. They can be written as follows.

$$N_1 = N_2 = N_1' = N_2' = 0, \qquad P = P_0 = x^{p_1} y^{p_2},$$

where

$$\gamma_1 = 2p_2 + 1, \qquad \gamma_2 = 2p_1 + 1, \qquad E = \tfrac{1}{2}(\omega_1 \gamma_2 + \omega_2 \gamma_1); \tag{9}$$

$$N_1 = N_2' = 1, \qquad N_2 = N_1' = 0,$$

$$P = [(C_2(0) - C_1(0))/(4\omega) + (x^2 - y^2)]P_0,$$

where

$$\gamma_1 = 2p_2 + 1, \qquad \gamma_2 = 2p_1 + 1, \qquad \omega_1 = \omega_2 = \omega, \qquad E = \tfrac{1}{2}\omega(\gamma_1 + \gamma_2 + 4); \tag{10}$$

$$N_1 = N_2 = 1, \qquad N_1' = 0, \qquad N_2' = 2,$$

$$P = [C_2(0)/(4\eta) - y^2(x^2 - y^2 + 2\omega/\eta)]P_0,$$

where

$$\begin{aligned} &\gamma_1 = 2p_2 + 5, \qquad \gamma_2 = 2p_1 + 1, \\ &\omega_1 = \omega_2 = \omega = [\eta(C_2(1) - C_1(0))/8]^{1/2}, \qquad E = \tfrac{1}{2}\omega(\gamma_1 + \gamma_2 + 4); \end{aligned} \tag{11a}$$

$$N_1' = N_2' = 1, \qquad N_1 = 2, \qquad N_2 = 0,$$

$$P = [C_1(0)/(4\eta) - x^2(y^2 - x^2 + 2\omega/\eta)]P_0, \tag{11b}$$

where

$$\gamma_1 = 2p_2 + 1, \qquad \gamma_2 = 2p_1 + 5,$$

$$\omega_1 = \omega_2 = \omega = [(C_1(1) - C_2(0))\eta/8]^{1/2}, \qquad E = \tfrac{1}{2}\omega(\gamma_1 + \gamma_2 + 4);$$

$$N_1' = N_2 = 1, \qquad N_1 = N_2' = 2,$$

$$P = (y^2 - x^2))[C_2(0)/(4\eta) - (xy)^2]P_0, \tag{12}$$

where

$$p_1 = p_2, \qquad \gamma_1 = \gamma_2 = 2p_1 + 5,$$

$$\omega_1 = \omega_2 = 0, \qquad E = 0.$$

This solution does not represent a bound state because for $\omega_i = 0$ the wavefunction $\psi(x, y)$ is not normalisable.

For $N_1' = N_2 = 0$, $N_1 = N_2' = 2$ the solution does not exist.

We obtained a finite class of the solutions of the Schrödinger equation for ACO with Hamiltonian (2), and for one set of the parameters λ_i, η we obtained only one state.

Let us consider the interesting case when the following assumption is made: $\omega_i^2 = \eta\gamma_i$. Then, the potential of ACO takes the form

$$V(x, y) = 2\eta(xy)^2[\nu + \tfrac{1}{2}\eta(x^2 + y^2)].$$

This potential becomes zero on the lines $x = 0$, $y = 0$ so it can be supposed that the bound states do not exist since unlimited classical motion along these can occur. The bound states do exist, however, if only $\eta > 0$.

When $\omega_i^2 < \eta\gamma_i$, we have $\lambda_i < 0$ and so

$$\lim_{x^2\to\infty} V(x, 0) = \lim_{y^2\to\infty} V(0, y) = -\infty,$$

but in this case also the bound states exist. This unexpected finding can be explained as follows.

The wavepacket localised in the $V(x, y)$ potential well cannot spread to infinity along, let us say, the curve $x = 0$, since it must crowd through a gap which in the limit narrows to zero. Indeed,

$$\lim_{x^2\to\infty} V(x, y) = \begin{cases} 0 & \text{for } y = 0, \\ \infty & \text{for } y \neq 0. \end{cases}$$

Such a shape of the potential imposes the localisation of the wavefunction and assures its normalisability.

The method used in this work may be straightforwardly employed in obtaining the solutions of type (2) for multidimensional polynomial potentials.

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