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Symmetries of the Jahn–Teller Systems and Their Solvability

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We present a method of obtaining the quasi-exact solution of the Jahn–Teller systems in the framework of $osp(2,2)$ superalgebra. The Hamiltonian have been solved in the Bargmann–Fock space by obtaining an expression as linear and bilinear combinations of the generators of $osp(2,2)$. In particular, we have discussed quasi-exact solvability of $E \times \varepsilon$ Jahn–Teller Hamiltonian.

1 Introduction

The Jahn–Teller (JT) distortion problem is an old one, dating back over sixty years [1]. Yet, even today, new contributions to this problem are being made [2]. They appear, however, not to have been fully exploited in the analysis of JT problem. The $E \otimes \varepsilon$ JT problem is a system with doubly degenerate electronic state and doubly degenerate JT active vibrational state. The JT effect describes the interaction of degenerate electronic states through non-totally symmetric, usually non-degenerate, nuclear modes. This effect plays an important role in explaining the structure and dynamics of the solids and molecules in degenerate electronic states.

The studies of the JT effect led Judd to discover a class of exact isolated solutions of the model [2]. The complete description of these solutions have been given by Reik et al [3]. They observed that the isolated solutions could be obtained by using Neumann series of expansions of the eigenvectors in the Bargmann–Fock space described by the boson operators. The same problem has been treated in [4].

On the other hand, the concept of quasi-exactly solvable (QES) systems discovered [5, 7–9] in the 1980's, has received much attention in recent years, both from the viewpoint of physical applications and their inner mathematical beauty. The classification of the 2×2 matrix differential equations in one real variable possessing polynomial solution have been described [6, 10]. The relevant algebraic structure of the $E \otimes \varepsilon$ JT system is the graded algebra $osp(2,2)$ and in this poster, we present a quasi-exact solution of the $E \otimes \varepsilon$ JT Hamiltonian.

2 Symmetry properties of the $E \times \varepsilon$ Jahn–Teller system

In this section a group theoretical treatment of JT distortion, in general case of two-fold degenerate states of various groups is provided. The JT interaction matrices and surface energies have been obtained by using symmetry properties of the system [11]. Let us start by describing the Hamiltonian that generates $D^\ell \otimes D^\ell$ surface, where D^ℓ denotes the irreducible representation. The standard Hamiltonian may be written in the form

$$H = H_0 + H_{\mathrm{JT}}, \tag{1}$$

where H_0 describes free (uncoupled) electron/holes and their vibrational states and H_{JT} is the Jahn–Teller interaction Hamiltonian. It is known that the Hamiltonian of the JT coupling is invariant under the rotational operations of the $SO(3)$ group. The totally symmetric part of direct product of an irreducible representations of a finite group, which describes the properties of the JT system, can be expressed in the form of

$$\left[D^\ell \otimes D^\ell\right] = D^{\ell_1} \oplus D^{\ell_2} \oplus \cdots \oplus D^{\ell_n}, \tag{2}$$

where ℓ is the angular momentum quantum number. Decomposition of $\left[D^\ell \otimes D^\ell\right]$ implies that the JT Hamiltonian can be written in the following way

$$H_{JT} = H^{\ell_1} + H^{\ell_2} + \cdots + H^{\ell_n}, \tag{3}$$

where H^{ℓ_i} is the JT Hamiltonian and it is invariant under the symmetry operations of the corresponding finite group, for the $(2\ell+1)$-dimensional representation. As an example consider an icosahedral symmetric system. The symmetric part of the H_g interaction is given by

$$[H_g \otimes H_g] = A_g \oplus H_g \oplus (H_g \oplus G_g), \tag{4}$$

where A_g, H_g, and G_g are the irreducible representations of the icosahedral group I_h. Since I_h is a subgroup of $O(3)$ decomposition of the coupling of the $\ell = 2$ state can be written as

$$\left[D^2 \otimes D^2\right] = D^0 \oplus D^2 \oplus D^4 \tag{5}$$

and its Hamiltonian is given by

$$H_{JT} = H^0 + H^2 + H^4. \tag{6}$$

The Hamiltonians H^i must be separately invariant under the symmetry group I_h. The symmetric part contains the totally symmetric representation $H^0 = A_g$ can exactly be solved. Before going further we list the decomposition of the symmetric products of the $[E \otimes E]$ JT interaction and corresponding symmetry groups

$$\begin{array}{llll} O_h: & [E\otimes E] = A_{1g} \oplus E, & T_h: & [E\otimes E] = A_g \oplus E, \\ D_{2p}: & [E\otimes E] = A_1 \oplus E, & C_{2p}: & [E\otimes E] = A_1 \oplus E, \end{array}$$

where O_h, T_h, D_{2p} and C_{2p} denotes octahedral, tetrahedral, dihedral and cyclic groups, respectively. In the following section we discuss the construction of the $E \otimes \varepsilon$ JT Hamiltonian.

3 The $E \otimes \varepsilon$ Jahn–Teller Hamiltonian

The well-known form of the $E \otimes \varepsilon$ JT Hamiltonian describing a two-level fermionic subsystem coupled to two boson modes has been given by Reik [3]

$$H = a_1^+ a_1 + a_2^+ a_2 + 1 + \left(\tfrac{1}{2} + 2\mu\right)\sigma_0 + 2\kappa[(a_1 + a_2^+)\sigma_+ + (a_1^+ + a_2)\sigma_-], \tag{7}$$

where $\frac{1}{2} + 2\mu$ is the level separation, κ is the coupling strength. The Pauli matrices $\sigma_{\pm,0}$ are given by

$$\sigma_+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \qquad \sigma_- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{8}$$

The annihilation and creation operators, a_i and a_i^+ satisfy the usual commutation relations

$$[a_i^+, a_j^+] = [a_i, a_j] = 0, \qquad [a_i, a_j^+] = \delta_{ij}. \tag{9}$$

The number operator of the Hamiltonian (7), J_1, represents the angular momentum of the system and is given by

$$J_1 = a_1^+ a_1 - a_2^+ a_2 + \tfrac{1}{2}\sigma_0. \tag{10}$$

Note that J_1 commutes with H and the eigenvalue problem of the angular momentum part can be easily solved and it reads

$$J_1 \left|\psi\right\rangle_{j+\frac{1}{2}} = \left(j+\tfrac{1}{2}\right)\left|\psi\right\rangle_{j+\frac{1}{2}}, \qquad j = 0,1,2,\ldots \tag{11}$$

with the eigenfunctions

$$\left|\psi\right\rangle_{j+\frac{1}{2}} = (a_1^+)^j \phi_1(a_1^+a_2^+)\left|0\right\rangle\left|\uparrow\right\rangle + (a_1^+)^{j+1}\phi_2(a_1^+a_2^+)\left|0\right\rangle\left|\downarrow\right\rangle, \tag{12}$$

where $\left|0\right\rangle$ is the vacuum state for both bosons. Here $\left|\uparrow\right\rangle$ and $\left|\downarrow\right\rangle$ are the eigenstates of the σ_0, ϕ_1 and ϕ_2 are arbitrary functions of $a_1^+a_2^+$. Because the operators H and J_1 commute, the eigenfunctions (12) are also the eigenfunctions of the Hamiltonian (7). Therefore we can write the eigenvalue equation,

$$H\left|\psi\right\rangle_{j+\frac{1}{2}} = E\left|\psi\right\rangle_{j+\frac{1}{2}}, \qquad E = 2\epsilon + j + \tfrac{3}{2}. \tag{13}$$

The Hamiltonian H can be expressed in the Bargmann–Fock space by using the realizations of the bosonic operators

$$a_i^+ = z_i, \qquad a_i = \frac{d}{dz_i}, \qquad i = 1,2. \tag{14}$$

In this formulation, the Hamiltonian H consists of two independent sets of first-order linear differential equations. Substituting (12) and (14) into (7) and defining $\xi = z_1z_2$ one can obtain the following two linear differential equations satisfied by the functions ϕ_1 and ϕ_2:

$$\begin{aligned}
&\left[\xi\frac{d}{d\xi} - (\epsilon-\mu)\right]\phi_1 + \kappa\left[\xi\frac{d}{d\xi} + (\xi+j+1)\right]\phi_2 = 0,\\
&\kappa\left[\frac{d}{d\xi}+1\right]\phi_1 + \left[\xi\frac{d}{d\xi} - (\epsilon+\mu)\right]\phi_2 = 0.
\end{aligned} \tag{15}$$

These coupled differential equations represent the Schrödinger equation of the $E\otimes\varepsilon$ JT system in Bargmann's Hilbert space and its isolated exact solution have been obtained by Reik [3]. In this paper we follow a different strategy to solve the Hamiltonian (7) and we show that the Hamiltonian possesses $osp(2,2)$ symmetry.

4 Two-boson one fermion $osp(2,2)$ superalgebra

In order to construct $osp(2,2)$ superalgebra let us start by introducing three generators of the $su(1,1)$ algebra,

$$J_+ = a_1^+a_2^+, \qquad J_- = a_2a_1, \qquad J_0 = \tfrac{1}{2}\left(a_1^+a_1 + a_2^+a_2 + 1\right). \tag{16}$$

These are the Schwinger representation of $su(1,1)$ algebra and its number operator is given by,

$$N = a_1^+a_1 - a_2^+a_2 \tag{17}$$

which commutes with the $su(1,1)$ generators. The superalgebra $osp(2,2)$ might be constructed by extending $su(1,1)$ algebra with the fermionic generators. These are given by

$$V_+ = f^+a_2^+, \qquad V_- = f^+a_1, \qquad W_+ = fa_1^+, \qquad W_- = fa_2, \tag{18}$$

where f^+ and f are fermions and they satisfy the anticommutation relation

$$\left\{f,f^+\right\} = 1, \qquad f = \sigma_-, \qquad f^+ = \sigma_+, \qquad ff^+ - f^+f = \sigma_0. \tag{19}$$

The superalgebra $osp(2,2)$ can be constructed with the generators (16) and (18), as it is discussed in [12]. The total number operator J of the system and it is given by

$$J = \tfrac{1}{2}N + \tfrac{1}{2}\left(f^+ f - f f^+\right). \tag{20}$$

The generators of the $osp(2,2)$ superalgebra satisfy the following commutation and anticommutation relations:

$$\begin{aligned}
&[J_+, J_-] = -2J_0, \qquad [J_0, J_\pm] = \pm J_\pm, \qquad [J, J_\pm] = 0, \qquad [J, J_0] = 0,\\
&[J_0, V_\pm] = \pm\tfrac{1}{2}V_\pm, \qquad [J_0, W_\pm] = \pm\tfrac{1}{2}W_\pm, \qquad [J_\pm, V_\mp] = V_\pm, \quad [J_\pm, W_\mp] = W_\pm,\\
&[J, W_\pm] = -\tfrac{1}{2}W_\pm, \qquad [J, V_\pm] = \tfrac{1}{2}V_\pm, \qquad [J_\pm, V_\pm] = 0, \qquad [J_\pm, W_\pm] = 0,\\
&\{V_\pm, W_\pm\} = J_\pm, \qquad \{V_\pm, W_\mp\} = \pm J_0 - J, \qquad \{V_\pm, V_\pm\} = \{V_\pm, V_\mp\} = 0,\\
&\{W_\pm, W_\pm\} = \{W_\pm, W_\mp\} = 0.
\end{aligned} \tag{21}$$

The Hamiltonian of a physical system, with an underlying $osp(2,2)$ symmetry, has been expressed in terms of the operators of the corresponding algebra.

5 Transformation of the operators

Transformation of the fermion-boson representations of the $osp(2,2)$ algebra and its connection with the QES systems can be done by introducing the following similarity transformation induced by the metrics

$$S = (a_2^+)^{-a_1^+ a_1 - \sigma_+\sigma_-}, \qquad T = (a_2)^{a_1^+ a_1 + \sigma_+\sigma_-}. \tag{22}$$

These transformations lead to the single-variable differential realizations of the $osp(2,2)$ superalgebra. With the operator S, the generators of $osp(2,2)$ takes the form:

$$\begin{aligned}
&J'_+ = SJ_+S^{-1} = a_1^+, \qquad J'_- = SJ_-S^{-1} = a_1(a_2^+ a_2 + a_1^+ a_1 + \sigma_+\sigma_-),\\
&J'_0 = SJ_0S^{-1} = \tfrac{1}{2}\left(2a_1^+ a_1 + a_2^+ a_2 + 1 + \sigma_+\sigma_-\right), \qquad J' = SJS^{-1} = \tfrac{1}{2}(-a_2^+ a_2 - \sigma_-\sigma_+),\\
&V'_+ = SV_+S^{-1} = \sigma_+, \qquad V'_- = SV_-S^{-1} = \sigma_+ a_1,\\
&W'_+ = SW_+S^{-1} = \sigma_- a_1^+, \qquad W'_- = SW_-S^{-1} = \sigma_-(a_2^+ a_2 + a_1^+ a_1 + \sigma_+\sigma_-).
\end{aligned} \tag{23}$$

The representations (23) of $osp(2,2)$ can be characterized by a fixed number $a_2^+ a_2 = -j - 1$. Here j takes integer or half-integer values. Therefore the generators of the $osp(2,2)$ algebra can be expressed as single-variable differential equation in the Bargmann–Fock space and two-component polynomials of degree j and $j+1$ form a basis function for the generators of the $osp(2,2)$ algebra,

$$P_{n+1,n}(x) = \begin{pmatrix} x^0, x^1, \ldots, x^{n+1} \\ x^0, x^1, \ldots, x^n \end{pmatrix}. \tag{24}$$

The general QES operator can be obtained by linear and bilinear combinations of the generators of the $osp(2,2)$ superalgebra. Action of the QES operator on the basis function (24) gives us a recurrence relation, therefore, the wavefunction is itself the generating function of the energy polynomials. Under the transformation T the generators of the $osp(2,2)$ algebra take the form

$$\begin{aligned}
&J'_+ = TJ_+T^{-1} = a_1^+(a_1 a_1 + a_2^+ a_2 + 1 + \sigma_+\sigma_-), \qquad J'_- = TJ_-T^{-1} = a_1,\\
&J'_0 = TJ_0T^{-1} = \tfrac{1}{2}\left(2a_1^+ a_1 + a_2^+ a_2 + 1 + \sigma_+\sigma_-\right) \quad J' = TJT^{-1} = \tfrac{1}{2}\left(-a_2^+ a_2 - \sigma_-\sigma_+\right),\\
&V'_+ = TV_+T^{-1} = \sigma_+(a_2^+ a_2 + a_1^+ a_1 + 1 + \sigma_+\sigma_-), \qquad W'_+ = TW_+T^{-1} = \sigma_- a_1^+,\\
&V'_- = TV_-T^{-1} = \sigma_+ a_1, \qquad W'_- = TW_-T^{-1} = \sigma_-.
\end{aligned} \tag{25}$$

This realization can also be characterized by $a_2^+ a_2 = -j - 1$. The basis function of the realization is given by (24).

6 Solvability of the $E \otimes \varepsilon$ Jahn–Teller Hamiltonian

It will be shown that our approach is relatively very simple when compared to previous approaches. The Hamiltonian (7) can be expressed in terms of the generators of the $osp(2,2)$:

$$H = 2J_0 + \left(\tfrac{1}{2} + 2\mu\right)(2J - N) + 2\kappa\left[V_+ + V_- + W_+ + W_-\right]. \tag{26}$$

The general trend to solve a differential equation quasi-exactly is to express the differential equation in terms of the generators of a given Lie algebra having a finite dimensional invariant subspace and to use the algebraic operations. In the Bargmann–Fock space the Hamiltonian has two different realizations, under the transformations S and T. The first transformation by S leads to the following one-variable differential realization:

$$\begin{aligned} H_1 = {} & \left(2x\frac{d}{dx} - j + \sigma_+\sigma_-\right) - \left(\tfrac{1}{2} + 2\mu\right)\sigma_-\sigma_+ \\ & + 2\kappa\left[\sigma_+\left(1 + \frac{d}{dx}\right) + \sigma_-\left(x + x\frac{d}{dx} - j - 1 + \sigma_+\sigma_-\right)\right] \end{aligned} \tag{27}$$

and the second realization can be obtained by transforming the Hamiltonian by T:

$$\begin{aligned} H_2 = {} & \left(2x\frac{d}{dx} - j + \sigma_+\sigma_-\right) - \left(\tfrac{1}{2} + 2\mu\right)\sigma_-\sigma_+ \\ & + 2\kappa\left[\sigma_+\left(\frac{d}{dx} + x\frac{d}{dx} - j + \sigma_+\sigma_-\right) + \sigma_-(1 + x)\right]. \end{aligned} \tag{28}$$

The eigenvalue problem can be expressed as

$$H\varphi(x) = E\varphi(x), \qquad \varphi(x) = \begin{bmatrix} v_n(x) \\ \omega_m(x) \end{bmatrix}, \tag{29}$$

where $v_n(x)$ and $\omega_m(x)$ are polynomials of degree n and m respectively. The action of the H_1 on the basis function $\varphi(x)$ gives the following recurrence relation:

$$\begin{aligned} & (2n - j + 1 - E)v_n + 2\kappa(\omega_m + m\omega_{m-1}) = 0, \\ & \left(2m - j - \tfrac{1}{2} - 2\mu - E\right)\omega_m + 2\kappa(v_{n+1} + (n - j)v_n) = 0. \end{aligned} \tag{30}$$

Similarly when the Hamiltonian H_2 acts on the basis function we obtain the recurrence relation:

$$\begin{aligned} & (2n - j + 1 - E)v_n + 2\kappa(m\omega_{m-1} + (m - j)\omega_m) = 0, \\ & \left(2m - j - \tfrac{1}{2} - 2\mu - E\right)\omega_m + 2\kappa(v_n + v_{n+1}) = 0. \end{aligned} \tag{31}$$

It is requiring that the determinant of these sets must be equal to zero giving the compatibility conditions which establish the QES system. According to the (24) one can construct a QES system if $n = m + 1$. Here m takes the values $m = 0, \frac{1}{2}, 1, \ldots, j$. If E_j is a root of the recurrence relations (30) or (31) then the eigenfunction truncates for a certain values of j, and E_j belong to the spectrum of the Hamiltonian. The initial conditions of the recurrence relation is given by

$$v_m = 0 \quad \text{for} \quad j < m < 1 \qquad \text{and} \qquad \omega_m = 0 \quad \text{for} \quad j < m < 0. \tag{32}$$

with these initial conditions solution of (30) gives us the following relation for the energy when $j = 0$:

$$E = \tfrac{1}{4}\left(5 - 4\mu \pm \sqrt{64\kappa^2 + (7 + 4\mu)^2}\right) \tag{33}$$

and for $j = 1/2$:

$$E = \tfrac{1}{4}\left(3 - 4\mu \pm \sqrt{32\kappa^2 + (7 + 4\mu)^2}\right), \qquad E = \tfrac{1}{4}\left(7 - 4\mu \pm \sqrt{64\kappa^2 + (7 + 4\mu)^2}\right). \tag{34}$$

The same energy eigenvalues can be obtained by using the recurrence relation (31). In this case eigenvalues shifted $E \to E - 1$ and j takes negative integer and half-integer values.

7 Conclusion

It is well known that the exact solutions have a direct practical importance. We have presented the quasi-exact solution of the generalized $E \otimes \varepsilon$ JT system. Our paper gives a unified treatment of some earlier works. The method given here can be extended to other JT or multi-dimensional atomic systems. The basic features of our approach is to construct $osp(2,2)$ invariant subspaces. Furthermore, we have presented two different boson-fermion representations and two classes of one variable differential realizations of $osp(2,2)$ algebra. In particular the solution of $E \otimes \varepsilon$ JT system has been constructed.

The suggested approach can be generalized in various directions. Invariant subspaces of the multi-boson and multi-fermion systems can be obtained by extending the method given in this paper. The method given here can be extended to other JT or multi dimensional atomic systems.

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