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Parabosons versus supersymmetry in Jahn–Teller systems

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Abstract. The applications of parabosons by Schmutz and of supersymmetry by Jarvis and Stedman in Jahn–Teller systems are compared and contrasted. Although a parasupersymmetric Jahn–Teller system has not yet been identified, the method of Schmutz is used here to show that the $E \times \epsilon$ supersymmetric Jahn–Teller Hamiltonian can be written in terms of paraboson operators.

1. Introduction

Jahn–Teller systems are interesting candidates for non-relativistic applications of supersymmetry in quantum mechanics because of the degeneracy of the fermion states, the existing fermion–boson interactions and the well established tradition for applying higher group symmetries to reveal approximate underlying symmetries (for example, Pooler and O'Brien 1977, Judd 1982, Stedman 1983).

The work of Schmutz (1980) on parabosons and that of Jarvis and Stedman (1984) on supersymmetry, respectively, in $E \otimes \epsilon$ Jahn–Teller Hamiltonians have superficially common features. We show that, although the differences in these approaches are fundamental and do not allow the identification of a parasupersymmetric Jahn–Teller system at this stage, the anharmonic terms introduced by Jarvis and Stedman to achieve supersymmetry may be given elegant representation using paraboson operators.

We take the Hamiltonian to be $H \equiv H_l + H_e + H_c + H_a$ where H_e, H_l are the unperturbed Hamiltonians of the N-fold degenerate electronic system and of a harmonic oscillator with the same degeneracy (so that supersymmetry is possible), H_c is the fermion–boson coupling term and H_a represents anharmonic phonon coupling. In the schemes of Jarvis and Stedman (1984), it is vital that anharmonic (boson–boson) couplings in H_c be present to act as the supersymmetric counterparts of the fermion–boson couplings under fermion–boson transmutations. Since physical systems will certainly possess some anharmonicity, this supersymmetric model is expected to be at least as realistic as those assuming harmonic couplings when discussing higher symmetry in Jahn–Teller systems.

In the $E \otimes \epsilon$ system, a doubly degenerate vibrational mode (of symmetry ϵ in, say, the group O) is vibronically coupled to a twofold-degenerate (E) electronic level ($H_e = 1$). The fermion–boson coupling has the form $H_c \equiv \sigma_z\phi_1 + \sigma_x\phi_2$, where $\phi_i = b_i + b_i^\dagger$, b_i and f_i are annihilation operators for boson mode and fermion state i, respectively, and σ_z and σ_x are the usual Pauli matrices. We shall write b, f for the associated column matrices (b_i), (f_i).

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2. Supersymmetry in Jahn–Teller systems

We now review and adapt the results of the Jarvis and Stedman formalism. The generator of supersymmetric transformations is the supercharge $S \equiv f^\dagger \cdot \beta$, where $\beta \equiv \exp G(\phi) b \exp(-G(\phi))$, $\phi \equiv \{\phi_i\}$, $i = 1, 2$, and G is any real differentiable function of ϕ. Therefore

$$[\overleftarrow{\beta}, \overrightarrow{\beta}] = 0 \qquad [\overleftarrow{\beta}, \overrightarrow{f^\dagger}] = [\overleftarrow{\beta}, \overrightarrow{f}] = 0$$

where the left and right arrows indicate row and column labels, respectively. S is nilpotent and the Hamiltonian $H = \{S, S^\dagger\}$ is necessarily supersymmetric (Witten 1982, Blockley and Stedman 1985, Stedman 1985).

We may expand β in terms of repeated commutators and use the result $[G(\phi), b_i^{(\pm)}] = \pm G^{(i)}(\phi)$, where the superscript i denotes a partial derivative with respect to ϕ_i. Since any two functions of ϕ commute we have $\beta = b - G'(\phi)$. It follows that

$$[\overleftarrow{\beta}, \overrightarrow{\beta^\dagger}] = 1 - 2G''(\phi).$$

The Hamiltonian becomes

$$\begin{aligned} H &= f^\dagger[\overleftarrow{\beta}, \overrightarrow{\beta^\dagger}]f + \beta^\dagger\beta \\ &= f^\dagger f + b^\dagger b - 2f^\dagger G''(\phi) f - G'(\phi) b - b^\dagger G'(\phi) + G'(\phi)^2. \end{aligned} \tag{1}$$

This may be written as $H = H_e + H_l + H_c + H_a$, where $H_c = -2f^\dagger G''(\phi) f$ and

$$\begin{aligned} H_a &= -G'(\phi)b - b^\dagger G'(\phi) + G'(\phi)^2 \\ &= \operatorname{tr} G''(\phi) - (G'(\phi))^{\mathrm{T}}\phi + G'(\phi)^2. \end{aligned} \tag{2}$$

Jarvis and Stedman point out that each such term in H is guaranteed to be invariant under the point group if the fermions and bosons transform in the same manner and if $G(\phi)$ is an invariant function; this follows since $\beta \sim b \sim f$ and a contraction such as $f^\dagger\beta$ is then invariant under the point group.

For the $E \otimes \epsilon$ Jahn–Teller system, Jarvis and Stedman (1984) choose a $D_4 \supset D_2$ subgroup basis so that $\phi = (\phi_1, \phi_2)^{\mathrm{T}} \sim ((3z^2 - r^2)/\sqrt{3}, x^2 - y^2)^{\mathrm{T}}$. The only quadratic, cubic and quartic invariants that can be constructed from ϕ are $I_2 \equiv (\phi_1^2 + \phi_2^2)$, $I_3 \equiv (\phi_1^3 - 3\phi_1\phi_2^2)$ and $I_4 \equiv I_2^2$. Also $\Phi \equiv (\phi_1^2 - {\phi_2}^2, -2\phi_1\phi_2)^{\mathrm{T}}$ transforms as ϕ. If $G_E \equiv -\frac{1}{3}\alpha I_3$ then $\beta = b + \alpha\Phi$ and

$$\begin{aligned} H_c &= -2f^\dagger \begin{pmatrix} -2\alpha\phi_1 & 2\alpha\phi_2 \\ 2\alpha\phi_2 & 2\alpha\phi_1 \end{pmatrix} f \\ &= 4\alpha(\phi_1(f_1^\dagger f_1 - f_2^\dagger f_2) - \phi_2(f_1^\dagger f_2 - f_2^\dagger f_1)) \\ &= 4\alpha f^\dagger(\phi_1\sigma_z - \phi_2\sigma_x) f. \end{aligned} \tag{3}$$

G_E generates a mixture of cubic and quartic anharmonicity: $H_a = \alpha I_3 + \alpha^2 I_4$. Thus

$$H_{\mathrm{JS}} = H_2 + H_e + H_c + H_a = b^\dagger b + f^\dagger f + 4\alpha f^\dagger(\phi_1\sigma_z - \phi_2\sigma_x) f + \alpha I_3 + \alpha^2 I_4. \tag{4}$$

On projecting out the fermion operators $H_{\mathrm{JS}} \to \boldsymbol{H}_{\mathrm{JS}}$ by the relation $H_{\mathrm{JS}} \equiv f^\dagger \boldsymbol{H}_{\mathrm{JS}} f$, we find

$$\begin{aligned} \boldsymbol{H}_{\mathrm{JS}} &= [\overleftarrow{\beta}, \overrightarrow{\beta^\dagger}] + (\beta^\dagger\beta)\mathbf{1} \\ &= (b^\dagger b + 1 + \alpha I_3 + \alpha^2 I_4)\mathbf{1} + 4\alpha(\phi_1\sigma_z - \phi_2\sigma_x). \end{aligned} \tag{5}$$

3. Parabosons in Jahn–Teller systems

Similarly, we briefly review and adapt the representation by Schmutz (1980) of an $E \otimes \epsilon$ Jahn–Teller system in terms of displaced parabose oscillators (we use $\alpha = \lambda/4$ and $\phi_2 \to -\phi_2$). Schmutz begins with the $E \otimes \epsilon$ Jahn–Teller Hamiltonian $\boldsymbol{H}_2 + \boldsymbol{H}_e + \boldsymbol{H}_c$:

$$\boldsymbol{H}_S = (\boldsymbol{b}^\dagger \boldsymbol{b} + 1)\mathbf{1} + 4\alpha(\phi_1 \sigma_z - \phi_2 \sigma_x) = (\boldsymbol{b}^\dagger \boldsymbol{b})\mathbf{1} + [\overleftarrow{\beta}, \overrightarrow{\beta^\dagger}]. \tag{6}$$

Note the omission of anharmonicity. The operator $\Gamma_i \equiv \exp(\mathrm{i}\pi b_i^\dagger b_i)$ and has the useful properties $\Gamma_i^\dagger = \Gamma_i^{-1}$, $\{\Gamma_i, b_i\} = 0$ and $\Gamma_i |n_i\rangle = (-1)^{n_i} |n_i\rangle$; in addition, since Γ_i^2 has expectation value unity in any space of definite (integer) number and commutes with all operators in the theory, we can take $\Gamma_i = \Gamma_i^\dagger = \Gamma_i^{-1}$ in all relations. A derived unitary operator $\boldsymbol{U}_1$ diagonalizes $\boldsymbol{H}_S$:

$$\boldsymbol{U}_i = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \Gamma_i \\ 1 & -\Gamma_i \end{pmatrix} \qquad \boldsymbol{H}_{S'} = \boldsymbol{U}_1 \boldsymbol{H}_S \boldsymbol{U}_1^\dagger = \begin{pmatrix} H_- & 0 \\ 0 & H_+ \end{pmatrix} \tag{7}$$

$$H_\eta \equiv \boldsymbol{b}^\dagger \boldsymbol{b} + 1 + 4\alpha(\phi_1 + \eta \phi_2 \Gamma_1) \tag{8}$$

where $\eta = \pm$. The operators $a_i, a_i^\dagger$, where $a_i \equiv b_i \Gamma_{3-i}$, $i = 1, 2$, obey boson commutation relations amongst themselves (as do $b_i, b_i^\dagger$), but each has a zero anticommutator with each of $b_i, b_i^\dagger$. $\boldsymbol{A} \equiv (A_+, A_-)^{\mathrm{T}} = \boldsymbol{U}_1 \boldsymbol{b}$, $A_\eta \equiv (b_1 + \eta a_2)/\sqrt{2}$. These operators satisfy the trilinear commutation relations characteristic of all $p = 2$ parabosonic operators (where ζ, like η, is either $+$ or $-$) (see for related material Green 1953, Greenberg and Messiah 1965, Rubakov and Spironodov 1988, Beckers and Debergh 1990a,b, Bardakci 1992):

$$[\{A_\eta, A_\eta^\dagger\}, A_{-\eta}] = -A_{-\eta} \qquad [\{A_\eta, A_\eta\}, A_\eta^\dagger] = 2A_\eta \qquad [\{A_\eta, A_\eta\}, A_\zeta] = 0. \tag{9}$$

Other such relations follow by Hermitian conjugation and also by the generalized Jacobi identity. $A_\pm$ may be defined by the relations $[N_\zeta, A_\eta] = -A_\eta$, where $N_\zeta \equiv \{A_\zeta, A_\zeta^\dagger\}$. In the two-dimensional case, $N_+ = N_- \equiv N$ and is the number operator for the system. The unperturbed Hamiltonian of the two-dimensional harmonic oscillator $H_2 = \boldsymbol{b}^\dagger \boldsymbol{b} + 1$ may be written as $H_2 = N = \boldsymbol{A}^\dagger \boldsymbol{A} + 1$. H_η can therefore be expressed as $H_\eta = N'_\eta - 16\alpha^2$, where $N'_\zeta \equiv \{A'_\zeta, A'^\dagger_\zeta\}$ and $A'_\eta \equiv A_\eta + 2\sqrt{2}\alpha$ so that $N'_\zeta = N + 2\sqrt{2}\alpha(A_\zeta + A_\zeta^\dagger) + 8\alpha^2$.

Hence, the Hamiltonians H_η are identical to those of the displaced parabose oscillators (A_η being the parabose operator and $2\sqrt{2}\alpha$ its displacement). Under the unitary transformation U_1 in which $\boldsymbol{H}_S \to \boldsymbol{H}'_S$, $\boldsymbol{f} \to \boldsymbol{f}'$ (which preserves the Fermi anticommutation relations) then $H_S = \boldsymbol{f}'^\dagger \boldsymbol{H}'_S \boldsymbol{f}'$, and parabosonic expressions are obtained in the Hamiltonian. The Schmutz diagonalization process may thus be viewed as a result of this unitary symmetry of the formalism.

4. Action of Schmutz transformations in the Jarvis and Stedman Hamiltonian

An obvious question is: what is the action of the Schmutz unitary diagonalizing matrix U_1 on the Jarvis and Stedman Hamiltonian $\boldsymbol{H}_{JS}$? Let $\boldsymbol{H}_{JS} \to \boldsymbol{H}'_{JS}$, $\boldsymbol{f} \to \boldsymbol{f}'$ and $\beta \to \beta'$ under $\boldsymbol{U}_1$. We obtain $\boldsymbol{H}'_{JS} = \boldsymbol{H}'_S + \alpha I_3 \sigma_x + \alpha^2 I_4 \mathbf{1}$. Since $H_{JS} = \boldsymbol{f}'^\dagger \boldsymbol{H}'_{JS} \boldsymbol{f}'$, this may be regarded as the original Hamiltonian in a unitarily transformed fermion basis. We note also that $S = f'^{\dagger}\beta'$, where $\beta' \equiv A + \alpha P_1$ and

$$P_1 \equiv \sqrt{2}\begin{pmatrix} C_-C_+ \\ C_+C_- \end{pmatrix}$$

with $C_\zeta \equiv A_\zeta + A_\zeta^\dagger$. Hence, S also involves paraboson operators and the (supersymmetric) Hamiltonian

$$H_{JS} = (f'^{\dagger}\beta')(\beta'^{\dagger} f') + (\beta'^{\dagger} f')(f'^{\dagger}\beta') = f'^{\dagger} H'_{JS} f'.$$

Since $b^\dagger b = A^\dagger A$

$$\beta'^{\dagger}\beta' = A^\dagger A + \alpha(A^\dagger P_1 + P_1^\dagger A) + \alpha^2 P_1^\dagger P_1 \tag{10}$$

$I_3 = \sqrt{2}(A^\dagger P_1 + P_1^\dagger A) = C_+C_-C_+$, $I_4 = P_1^\dagger P_1 = \{C_+C_-, C_-C_+\}$ and so the Jahn–Teller Hamiltonian may be written

$$H_{JS} = f'^{\dagger}(H_S + \alpha(P_1^\dagger A + A^\dagger P_1)\sigma_x + \alpha^2 P_1^\dagger P_1) f'. \tag{11}$$

At this point we simply follow Schmutz's method for rendering such a Hamiltonian diagonal, using the fermion transformation associated with U_2; and, as in the work of Schmutz, the effect is to further highlight the paraboson operators. If $U \equiv U_2U_1$, $H_{JS} \to H''_{JS}$, $f \to f''$ and $\beta \to \beta''$ under U then

$$H''_{JS} = (b^\dagger b + 1 + 4\alpha(\phi_1 - \phi_2\Gamma_1))1 + \alpha I_3\Gamma_2\sigma_z + \alpha^2 I_4 1 = \begin{pmatrix} H_{JS+} & 0 \\ 0 & H_{JS-} \end{pmatrix} \tag{12}$$

where

$$\begin{aligned} H_{JS\eta} &= b^\dagger b + 1 + 4\alpha(\phi_1 - \phi_2\Gamma_1) + \eta\alpha I_3\Gamma_2 + \alpha^2 I_4 \\ &= (N'_- - 16\alpha^2 + \alpha^2 I_4)1 + \eta\alpha I_3\Gamma_2 \end{aligned} \tag{13}$$

or, in terms of paraboson operators,

$$H_{JS} = (N'_- - 16\alpha^2)1 + \alpha(P_1^\dagger A + A^\dagger P_1)\Gamma_2\sigma_z + \alpha^2(P_1^\dagger P_1)1.$$

Hence

$$H_{JS} = f''^{\dagger}(U[\overleftarrow{\beta}, \overrightarrow{\beta^\dagger}]U^\dagger + U\beta''^{\dagger}\beta'' U^\dagger) f''. \tag{14}$$

It is instructive to write in the last term

$$\beta''^{\dagger}\beta'' = \beta^\dagger(\Gamma_2U_2)^\dagger(\Gamma_2U_2)\beta = b^\dagger b + \alpha(B^\dagger P_2 + P_2^\dagger B)\Gamma_2 + \alpha^2 P_2^\dagger P_2 \tag{15}$$

where

$$B \equiv \begin{pmatrix} B_+ \\ B_- \end{pmatrix} = \Gamma_2U_2 b \qquad P_2 \equiv U_2\Phi = \sqrt{2}\begin{pmatrix} D_+D_- \\ D_-D_+ \end{pmatrix}$$

$$D_\zeta \equiv B_\zeta + B_\zeta^\dagger \qquad B_\zeta \equiv (b_1\Gamma_2 + \zeta b_2)/\sqrt{2}.$$

$\{B_\xi\}$ are therefore paraboson operators (i.e. they obey a mixture of commutation and anticommutation relations). In addition $B^\dagger B = b^\dagger b = A^\dagger A$, $I_3 = (B^\dagger P_2 + P_2^\dagger B)\Gamma_2$, $I_3\Gamma_2 = \sqrt{2}(D_+D_-D_+ + D_-D_+D_-)$ and $I_4 = P_2^\dagger P_2 = 2\{D_+D_-, D_-D_+\}$ so that

$$U\beta^\dagger\beta U^\dagger = A^\dagger A + \alpha(B^\dagger P_2 + P_2^\dagger B)\Gamma_2 + \alpha^2 P_2^\dagger P_2 \tag{16}$$

and thus

$$H_{JS}(A,B) = (N'_- - 16\alpha^2)1 + \alpha(P_2^\dagger B + B^\dagger P_2)\sigma_z + \alpha^2(P_2^\dagger P_2)1. \tag{17}$$

This is a diagonal Hamiltonian expressed entirely in terms of parabosons.

Remarkably, the anharmonic terms are very amenable to expression in terms of paraboson operators. The cubic and quartic anharmonicity invariants I_3 and I_4 have, in fact, a far more elegant relationship when so expressed; the symmetry between the plus and minus parabosons is manifest.

5. Parasupersymmetry?

All of the former analysis is confined to standard fermi–bose supersymmetry, the generator and spectrum of which are reported in Jarvis and Stedman (1984). However, the above analysis is suggestive of a role for parasupersymmetry in Jahn–Teller theory.

The usual approach, however, is to use parafermi–bose supersymmetry (Jarvis 1978, Rubakov and Spiridonov 1988, Beckers and Debergh 1990a). This can lead to spectra with threefold degeneracies. Such a possibility of alternative higher symmetries would continue and enhance the above-mentioned tradition for applying higher group symmetries in Jahn–Teller systems.

Following the first example of Rubakov and Spiridonov (1988) we might search for parasupersymmetry using the paracharge

$$Q = \begin{pmatrix} 0 & 0 & 0 \\ p + \mathrm{i}W_1 & 0 & 0 \\ 0 & p + \mathrm{i}W_2 & 0 \end{pmatrix}$$

leading to a Hamiltonian of the form

$$H = \tfrac{1}{2}p^2 + W_1^2 + W_2^2 + \tfrac{1}{3}(W_1' - W_2') + \tfrac{1}{3}\begin{pmatrix} 2W_1' + W_2' & 0 & 0 \\ 0 & W_2' - W_1' & 0 \\ 0 & 0 & -W_1' - 2W_2' \end{pmatrix}.$$

For this to replicate, say the $T \times \epsilon$ Jahn–Teller system, we need to identify this interaction by an appropriate choice of the superpotentials W_1, W_2. The $T \times \epsilon$ Jahn–Teller system has an interaction, when diagonalized, of the form

$$\begin{pmatrix} \sqrt{\phi_1^2 + \phi_2^2} & 0 & 0 \\ 0 & -\sqrt{\phi_1^2 + \phi_2^2} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Hence, we would have to identify

$$2W_1' + W_2' = W_1' - W_2' = 3W_1'/2 = \sqrt{\phi_1^2 + \phi_2^2} \qquad W_1' = -2W_2'.$$

While these relations are algebraically consistent, each potential must contain both ϕ_1 and ϕ_2; in addition, the further conditions required by Rubakov and Spiridonov give the unlikely requirement that $W_2'(W_2 {}^+_- 2W_1) = 3W_2''$. This approach therefore seems unpromising. Nevertheless the paraboson link established here may help to indicate a better direction for studying possible realizations of parasupersymmetric systems.

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