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Supersymmetry in Jahn–Teller systems

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Abstract. Supersymmetric Hamiltonians are constructed for $E\otimes\varepsilon$ and $T\otimes\tau$ Jahn–Teller systems in octahedral symmetry. These represent a new class of Jahn–Teller Hamiltonians with a higher continuous symmetry, since they necessarily include anharmonic couplings among the vibrational modes. In such applications, supersymmetry has the physical consequences of relating Jahn–Teller energies to purely anharmonic energy shifts of pure vibrational states, and of relating Ham reduction factors to anharmonic dressing or renormalisation of the matrix elements of a vibrational operator. In each of the above systems a supergroup classification scheme is used to assign levels, and perturbation calculations are made of Ham reduction factors and the associated anharmonic renormalisation effects.

1. Introduction

Since the discovery of the possibility of supersymmetry, or invariance under boson–fermion mixing, in physical theories, many supersymmetric models have been discussed in the context of relativistic field theory and supergravity. Our aim will be to construct and investigate similar models in a non-relativistic theory with applicability to existing topics in condensed matter theory, and in particular to Jahn–Teller active systems.

Early non-relativistic applications of supersymmetry (e.g. Nicolai 1976) involved supersymmetric Hamiltonians of a relatively simple type. More recently superfield formulations have found applicability in the theory of the transport properties of alloys (Efetov 1983).

A more useful lead for our work is furnished by Witten (1981) who described models in supersymmetric quantum mechanics, i.e. field theories in $0+1$ dimensions. Such models have been derived from the superfield formalism of Salam and Strathdee (1975) by restricting to one dimension (Cooper and Freedman 1983).

In Jahn–Teller active systems, the electronic states of interest are the orbitally degenerate states of a substitutional ion, the boson modes are the vibrations of the surrounding ligands, and the interaction terms in the Hamiltonian correspond to the coupling of electronic and vibrational states and also to anharmonic effects amongst the vibrational modes.

Higher continuous symmetries have found a special importance in the discussion of properties of a Jahn–Teller system. Judd (1982) has reviewed the application of Lie groups, particularly $O(n)$, with $n=2, 3, 4, 5$, to various Jahn–Teller systems; a simple tetragonal example is discussed by Stedman (1984). Judd (1984) has described the interest of such higher symmetries as enormous.

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In all such cases of higher symmetry, the generators correspond to transformations in which the electronic states are mixed amongst themselves, while simultaneously but separately the vibrational states are mixed among themselves. To achieve invariance of the Hamiltonian under such operations, it is usually necessary to restrict the possible terms in the interaction severely. Only linear coupling of the electronic states with the vibrations is permitted, and if more than one vibrational level is involved, only one vibrational frequency and one coupling constant (the 'equal coupling' constraint) is allowed. Nevertheless the resulting Hamiltonian may prove to be a reasonable first approximation for a given system (e.g. F^+: CaO; for references see Judd (1984)). The higher symmetry may then permit analytic calculations which act as mileposts in a more refined, if numerical, approach in which the constraints associated with the higher symmetry are avoided. Even when the higher symmetry is badly broken in practice, it is formally advantageous in a symmetry-related problem to use the greatest available chain of groups for classification. The manner of breaking of a higher symmetry may itself give useful information, as in particle physics.

It is both natural and desirable, then, to consider extensions of such higher symmetries. If we relax the requirement that electronic and vibrational states should transform separately, we are led to consider the possibility of constructing supersymmetric Jahn–Teller Hamiltonians. In this paper, we demonstrate the possibility and utility of this extension. We also demonstrate the application in this context of recent advances in the analysis of supergroups and their branching rules.

Some consequences of supersymmetry are obvious at this stage. First, if bosons and fermions are to intermingle, we must require the same number of each (Witten 1981). This immediately suggests that for octahedral symmetry the $E\otimes\varepsilon$ and $T\otimes\tau$ systems (in which fermions and bosons both form doublets and triplets respectively) are of particular interest. We note (cf §§ 3.1, 3.2.2) that while it is convenient to choose such systems in which bosons and fermions transform similarly, it is not necessary; indeed, the ideas of N-extended supersymmetry and of the Wess–Zumino model (Wess and Zumino 1974), reduced to one dimension, each suggest the possibility of models in which for example a doublet fermion is coupled in a supersymmetric manner to two scalar bosons. However, the $E\otimes\varepsilon$ and $T\otimes\tau$ systems will be adequate illustrations.

Second, the energies of all bosons must be equal, as in the higher symmetry models referred to above; in addition, this energy must equal that of all the fermions. (The degeneracies associated with supersymmetry must hold at zero order of the perturbations.) Within one level, which is all that we shall consider, the electronic states certainly have the same energy, and it is only a formal constraint to require this energy to match the common vibrational energy. We may anticipate here one result of our analysis (§ 5.1); the restriction to a single mode frequency is known to necessitate certain sum rules between the Ham reduction factors up to at least fourth order in perturbation (Payne and Stedman 1983c).

Third, there must be anharmonic terms present in the interaction. The linear electron–vibration (or Jahn–Teller) coupling is quadratic in the fermion and linear in the boson operators (equation (16)); under replacement of a fermion by a boson operator, we may expect to generate cubic terms in boson operators. This represents a new departure in Jahn–Teller theory. There has been considerable interest in the inclusion of anharmonic effects in Jahn–Teller theory (e.g. Bates 1978), and a systematic perturbative method for their inclusion has been developed by Payne and Stedman (1983a). The prospect of a model which includes anharmonicity and yet possesses a

higher symmetry has much appeal, and could conceivably have a similar practical importance as a case study in the anharmonic regime to that of the more conventional higher symmetry models in the linear coupling regime. The strength of the allowed anharmonicity is of course highly constrained, since it mixes with the linear coupling under a supersymmetry transformation.

Fourth, all these interactions are also constrained by the nature of the physical application; in particular, they must be invariants under the point group operations. This invariance, together with some important consequences, has been emphasised by Ham (1965). It may not be superfluous to re-emphasise that in the absence of cooperative effects, etc, Jahn–Teller systems satisfy all point group symmetry requirements, despite the notorious breakdown of symmetry associated with the names of Jahn and Teller. Supersymmetry is as compatible with these requirements as it is with the internal symmetries encountered in particle physics applications (Salam and Strathdee 1975). In fact, it is easy to construct supersymmetric Jahn–Teller Hamiltonians; one need only ensure that the supersymmetric charges (or generators) transform irreducibly under the point group, and then construct the Hamiltonian as their invariant square. A reasonably general prescription for this procedure is given and illustrated in § 3.1. Since the symmetry aspects of such constructions are familiar to experimenters as well as to theorists in this area of condensed matter physics, we consider the Jahn–Teller application of supersymmetry to be particularly instructive.

Fifth, supersymmetry will forge relationships (§§ 4.4, 5.2) between the properties of one-fermion, zero-boson and zero-fermion, one-boson states and thus between parameters associated with the Jahn–Teller active ion, such as the Ham reduction factors (Ham 1965), and parameters associated with the vibrations alone. Again this represents a new departure in Jahn–Teller theory, whose consequences will be investigated. We note that relationships involving multifermion states have no such physical interpretation; multifermion states are unphysical, in that an ion may occupy only one state at any time (§ 3.1).

How realistic is supersymmetry? Nature is under no obligation to furnish us with an approximate realisation of a supersymmetric Jahn–Teller system. There is no experimental evidence for supersymmetry in any field of physics at this stage; it is indeed certain only to be broken. The requirement that all vibrational frequencies should be identical itself prohibits an exact application to a crystal lattice, which possesses a broad frequency spectrum; as noted above, this very breadth has a characteristic qualitative effect on reduction factors. The same objection applies also to the conventional higher symmetries of the 'equal coupling' type. As mentioned above, this has not prevented an approximate physical realisation of such a symmetry in the F^+: CaO system, nor does it negate the formal value of a higher symmetry as an initial classification scheme etc.

Supersymmetry is certainly no less realistic than any of the conventional higher symmetries (§ 3.2.3) Anharmonicity is always present. In conventional higher symmetries, it is ignored; in our supersymmetric models, it is constrained by an equal-coupling condition which parallels exactly the equal coupling condition of several higher symmetry Jahn–Teller systems. The wide variety of Jahn–Teller systems now reported (e.g. Challis and de Göer 1983) indicates that such levels of anharmonic coupling are readily attainable in practice.

In § 2 we discuss some elementary ideas in supersymmetric quantum mechanics, with one boson and one fermion state as basis. In § 3 we generalise to doublets and triplets, and construct the $E\otimes\varepsilon$ and $T\otimes\tau$ supersymmetric Jahn–Teller Hamiltonians.

In § 4 an analysis in terms of supergroups is given to classify the eigenstates of the supersymmetric Jahn–Teller Hamiltonians, and their eigenvalues are evaluated to second order, illustrating the connection imposed by supersymmetry between Jahn–Teller energies of the one-fermion states on the one hand and anharmonic corrections to the energies of one-boson states on the other. In § 5 the Ham reduction factors for the supersymmetric Jahn–Teller Hamiltonians and their supersymmetric analogues—the effects of higher-order anharmonic dressing on vibrational transitional amplitudes—are discussed, and calculations are performed to fourth and to second order respectively.

2. Introductory applications

We adopt here a very elementary approach which does not assume previous knowledge of supersymmetry transformations. An essential feature of supersymmetric quantum mechanics is that a charge (or conserved quantity) exists which is equal to the square root of the Hamiltonian (Lancaster 1983).

Consider first the Hamiltonian

$$H_1 = f^+ f + b^+ b \tag{1}$$

where f, b are fermion and boson annihilation operators respectively. This Hamiltonian is almost trivially supersymmetric; this is indicated by its form and by the degeneracies of its eigenstates. (If $|B, F\rangle$ is the eigenstate with B bosons and F fermions present, the states $|B, 1\rangle$ and $|B+1, 0\rangle$ are degenerate.)

In this example the generators of supersymmetry transformations are

$$S_1 = f^+ b \tag{2}$$

(which obviously replaces a boson by a fermion) and its adjoint S_1^+. It is easily seen that $S_1^2 = 0$, and that if the self-adjoint charge is defined by $Q_1 = S_1 + S_1^+$, then $H_1 = Q_1^2 = \{S_1, S_1^+\}$. The supersymmetry itself ($[H_1, S_1] = 0$) then follows directly from a Jacobi identity amongst commutator ([ ]) and anticommutator ({ }) brackets:

$$[\{A, B\}, C] + [\{B, C\}, A] + [\{C, A\}, B] = 0 \tag{3}$$

where $A = B = S_1$, $C = S_1^+$.

This example is readily extended to N fermions and N bosons (e.g. Nicolai 1976), the Hamiltonian

$$H_N = \sum_{i=1}^{N} (f_i^+ f_i + b_i^+ b_i) \tag{4}$$

being invariant under the transformation generated by

$$S_N = \sum_{i=1}^{N} f_i^+ b_i. \tag{5}$$

The proof is carried out in the same manner; $S_N^2 = 0$, and so the construction $H_N = Q_N^2 = (S_N + S_N^+)^2$ guarantees supersymmetry through equation (3). In this example all states with the same total number of fermions and bosons are degenerate.

Of more interest are supersymmetric models which contain a linear interaction with the bosons as in the relativistic and field theoretic models (e.g. Salam and Strathdee

1975). Such models are illustrated by Witten (1981) (e.g. one may take $W(x) = -x + \alpha x^2$ in equation (3.2) of Cooper and Freedman (1983)). For example

$$H_I = f^+ f + b^+ b - 4\alpha f^+ f\phi + 2\alpha\phi - \alpha\phi^3 + \alpha^2\phi^4 \tag{6}$$

is supersymmetric with respect to the generator

$$S_I = f^+\beta \tag{7}$$

where

$$\beta \equiv b - \alpha\phi^2,\ \phi \equiv b + b^+.$$

The proof is most easily performed again by defining $Q_I \equiv S_I + S_I^+$, $H_I \equiv Q_I^2$; in particular

$$H_I = f^+ f[\beta, \beta^+] + \beta^+\beta. \tag{8}$$

A more general example may be found by using these definitions together with (7) and the definition $\beta = \exp G(\phi)\, b \exp(-G(\phi))$; $G(\phi)$ can be any real function of ϕ. (In the above example, $G(\phi) = \frac{1}{3}\alpha\phi^3$.) Note that since $\exp G(\phi)$ is non-unitary, β is not a boson operator, i.e. $[\beta, \beta^+] \neq 1$; it is just this fact which results in a linear coupling in equation (6).

As anticipated in the introduction, the supersymmetric Hamiltonian with a linear coupling term ($f^+ f\phi$) also contains cubic anharmonicity (ϕ^3). We note the presence of a quartic term (ϕ^4) at higher order; this is also a general feature. While confined to one fermion and one boson, this Hamiltonian is a prototype of the result that we seek.

It is a simple exercise in perturbation theory to show that to second order in α, the ground state $|0,0\rangle$ is unshifted and the eigenstates corresponding to $|B, 1\rangle$ and $|B+1, 0\rangle$ remain degenerate with the common energy

$$E_{B+1} = B + 1 - 24\alpha^2(B+1)^2 - 3\alpha^2. \tag{9}$$

The uniqueness and zero energy of the ground state, and two-fold degeneracy of all other states, are elementary consequences of the above algebraic structure of supersymmetric quantum mechanics (Lancaster 1983). The computation of perturbation expressions analogous to equation (9) in supersymmetric Jahn–Teller systems will be outlined in § 3.

3. Supersymmetric Jahn–Teller Hamiltonians

3.1. Introduction and general construction

We search for supersymmetric Hamiltonians with relevance to Jahn–Teller active systems. The implies that they should contain more than one fermion and boson (as H_N, equation (4)) as well as a linear coupling between them (as H_I, equation (6)), and that they should be invariant under the appropriate point group symmetry operations.

Fermions are naturally incorporated by identifying a one-fermion state $f_i^+|0\rangle$ as an ionic state $|i\rangle$, a member of the degenerate set under consideration. This identification is the basis of a particularly convenient quantum-field theoretic method, pioneered by Abrikosov (1965) for spin operators, and applied in Jahn–Teller theory by Gauthier and Walker (1976) and Payne and Stedman (1983a, b, c).

It might be objected that the statistics of the ionic levels is Maxwell–Boltzmann rather than Fermi–Dirac, the multi-fermion and zero-fermion states being unphysical.

However, as in the field theoretic method, the effects of unphysical states may be projected out (Abrikosov 1965).

A more serious objection is that since there is now a wide variety of adaptations of the standard field theoretic methods for spin systems, a bosonic analogue of the Abrikosov technique could be used, removing the motivation for the introduction of supersymmetry into Jahn–Teller theory. The prototype of (6) gives some insight here. We may define a 'bosonised' version of (6) for which $[f, f^+] = 1$; (8) still holds. However, it is difficult, perhaps impossible, to identify a continuous symmetry operation for this bosonised Hamiltonian for the following reasons. First, since β is not a boson operator, (7) is not a conventional canonical transformation for the bosonised case. Second, no combination of the operators $f\beta$, $f^+\beta$, $\beta^+ f$, $\beta^+ f^+$ commutes with the bosonised Hamiltonian. Third, the bosonised Hamiltonian has second-order eigenvalues in analogy to (9) of the form

$$E' = T + (8N'(N'-1) - 24T^2 - 3)\alpha^2$$

where $N' \equiv \langle f^+ f \rangle_0$, $T \equiv B + N'$. This necessarily shows the 'supersymmetry' degeneracy (E' depends on T only for $N' = 0, 1$), but no further degeneracies (in general E' depends on N' as well as T).

The unperturbed Hamiltonian is H_N (equation (4)), N being the number of fermion and of boson states. We generalise the method of § 2 by defining as generator of supersymmetric transformations

$$S \equiv \sum_{i=1}^{N} f_i^+ \beta_i, \tag{10}$$

$$\beta_i \equiv \exp G(\boldsymbol{\phi})\, b_i \exp -G(\boldsymbol{\phi}), \tag{11}$$

where $(\boldsymbol{\phi}) = (\phi_1, \phi_2, \ldots, \phi_N)$ and $\phi_i = b_i + b_i^+$, G being a real function as before. Hence

$$[\beta_i, \beta_j] = 0, \qquad [\beta_i, f_j^{(+)}] = 0 \tag{12}$$

and $S^2 = 0$ as required. We expand the exponentials in (11) in terms of repeated commutators. Since $[G(\boldsymbol{\phi}),\ b_i^{\pm}] = \pm G^{(i)}(\boldsymbol{\phi})$, the superscript i denoting a partial derivative with respect to ϕ_i, and since any two functions of $(\boldsymbol{\phi})$ commute, we have

$$\beta_i = b_i - G^{(i)}(\boldsymbol{\phi}), \tag{13}$$

$$[\beta_i, \beta_j^+] = \delta_{ij} - 2G^{(ij)}(\boldsymbol{\phi}). \tag{14}$$

The Hamiltonian is found by constructing the symmetric square of S and becomes

$$H = \sum_{ij} f_i^+ f_j [\beta_i, \beta_j^+] + \sum_i \beta_i^+ \beta_i = H_N + H_c + H_a, \tag{15}$$

$$H_c = -2 \sum_{ij} G^{(ij)}(\boldsymbol{\phi}) f_i^+ f_j = 2 \sum_i \beta_i^{(j)} f_i^+ f_j, \tag{16}$$

$$H_a = (\beta_i^+ \beta_i - b_i^+ b_i)$$

$$= \sum_i \{G^{(ii)}(\boldsymbol{\phi}) - G^{(i)}(\boldsymbol{\phi})\phi_i + [G^{(i)}(\boldsymbol{\phi})]^2\}$$

$$= \sum_i (\beta_i^{(i)} + \beta_i \phi_i + \beta_i^2), \tag{17}$$

where H_c represents the ion–vibration coupling, and H_a anharmonic couplings amongst the vibrations. Clearly if $G(\boldsymbol{\phi})$ contains a cubic term, H_c will contain a linear coupling, and H_a cubic and quartic terms. A quadratic coupling in H_c may be obtained from a quartic term in $G(\boldsymbol{\phi})$, etc.

We have chosen G to depend on the ϕ_i or position operators rather than the momentum operators $\pi_i = b_i - b_i^+$ so as to ensure that H_c and H_a involve the conventional electric, rather than magnetic, couplings to and among the vibrations.

By construction, the Hamiltonian H (equation (15)) is supersymmetric. It is also guaranteed to be invariant under the point group if the fermions and bosons, (f_i), (b_i), transform in the same manner, and if $G(\boldsymbol{\phi})$ is an invariant function. These conditions also guarantee that (β_i) and (b_i) transform in the same way, and that the generator S is an invariant. In short, supersymmetric Hamiltonians are readily constructed, the method requiring only a vibrational and invariant operator $G(\boldsymbol{\phi})$ as input.

It is not necessary that S be an invariant. An example is discussed in the $T_1 \otimes \tau_2$ system (§ 3.2.2). In general, one might use the fermion and boson operators to construct a set of generators $\{S_l^\lambda \,|\, l = 1, 2, \ldots, |\lambda|\}$ transforming as an irrep λ of the symmetry group, and then construct the invariant and supersymmetric Hamiltonian as $H = \Sigma_l \{S_l^\lambda, S_l^{\lambda +}\}$. This gives no new results in the cases discussed in § 3.2.

3.2. Octahedral examples

3.2.1. $N = 2$: $E \otimes \varepsilon$. In the $E \otimes \varepsilon$ system, fermions (f_i) and bosons (b_i) each form a doublet transforming as the E irrep of the group O. We choose a $D_4 \supset D_2$ subgroup basis, so that $(\phi_1, \phi_2) \sim ((1/\sqrt{3})(3z^2 - r^2), x^2 - y^2)$.

Elementary point group theory indicates that the only possible quadratic, cubic and quartic invariants that may be constructed from $(\boldsymbol{\phi})$ are

$$I_2 \equiv (\phi_1^2 + \phi_2^2), \qquad I_3 \equiv \phi_1^3 - 3\phi_1\phi_2^2, \qquad I_4 \equiv I_2^2; \tag{18}$$

in addition, that $(\boldsymbol{\Phi}) \equiv (\phi_1^2 - \phi_2^2, -2\phi_1\phi_2)$ also transforms as (ϕ_1, ϕ_2).

A supersymmetric Jahn–Teller Hamiltonian may readily be derived as follows. We define $G_E = -\frac{1}{3}\alpha I_3$, the numerical constant included only for later simplicity. This gives in (11)

$$\beta_i = b_i + \alpha \Phi_i. \tag{19}$$

From the above comments, this form could have been written down as an obvious symmetry-preserving extension of the operators b_i, without the need for reference to G_E. Equation (16) then gives as one component of the supersymmetric Hamiltonian the standard coupling in the $E \otimes \varepsilon$ system:

$$H_c^E \equiv 4\alpha[(f_1^+ f_1 - f_2^+ f_2)\phi_1 - (f_1^+ f_2 + f_2^+ f_1)\phi_2]. \tag{20}$$

Equation (17) gives a mixture of cubic and quartic anharmonicity (the invariants are defined in (18)):

$$H_a^E \equiv \alpha I_3 + \alpha^2 I_4. \tag{21}$$

The simplest supersymmetric Jahn–Teller Hamiltonian is then

$$H_E = H_2 + H_c^E + H_a^E \tag{22}$$

with the definitions of equations (4), (20), (21).

If I_4 were also included in G_E, one could as readily obtain a quadratic ion–vibration coupling and anharmonic terms up to sixth order; for simplicity we omit these.

3.2.2. $N=3$: $T\otimes\tau$. Let (f_i), (b_i), $i=1, 2, 3$, span the T_2 irrep of O, in the basis $D_3\supset C_3$, i.e. $\phi_1\sim x_2x_3$ etc. We have the lower-order invariants

$$J_2=\sum_{i=1}^{3}(\phi_i)^2, \qquad J_3=\phi_1\phi_2\phi_3, \qquad J_4=(\phi_2^2\phi_3^2+\phi_3^2\phi_1^2+\phi_1^2\phi_2^2) \tag{23}$$

and $(\boldsymbol{\Phi})\equiv(\phi_2\phi_3,\ \phi_3\phi_1,\ \phi_1\phi_2)$ also transforms as T_2 in this basis. The definition $G_T=-\alpha J_3$ produces equation (18) in this case also, and as before we derive the $T_2\otimes\tau_2$ supersymmetric Jahn–Teller Hamiltonian

$$H_T=H_3+H_c^T+H_a^T, \tag{24}$$

$$H_c^T=2\alpha[(f_2^+f_3+f_3^+f_2)\phi_1+et\ cyc], \tag{25}$$

$$H_a^T=3\alpha J_3+\alpha^2J_4. \tag{26}$$

The same construction applies to $T_1\otimes\tau_2$; here S (equation (10)) is now not an invariant, but transforms as the irrep A_2 of O. However, its symmetric square H_T is invariant since $A_2\otimes A_2=A_1$. The $T_1\otimes\tau_2$ and $T_2\otimes\tau_2$ Jahn–Teller systems are isomorphic.

3.2.3. Discussion. Once again, the strategy has been simply to write down a suitable generator (equation (10)) and to form its symmetric square. As the above derivations emphasise, the terms arising in the supersymmetric Hamiltonian are just and only those allowed by point group symmetry at any order. Supersymmetry merely constrains their relative magnitudes, and that absolutely. The appearance of fourth-order anharmonicity at second order in the parameter α has a commendable realism. It may be noted that this parallels exactly the fourth-order terms arising in the massive interacting Wess–Zumino model when the auxiliary fields are eliminated (Fayet and Ferrara 1977, p 270). This suggests that the auxiliary field formalism could find application in this context also; we have not explored this.

The relative magnitude of the anharmonic and linear couplings associated with these supersymmetric Jahn–Teller Hamiltonians has consequences for the Jahn–Teller effect and adiabatic energy surfaces in such systems. On inserting this relative magnitude into the equations of Bates (1978, p 261) we find that a supersymmetric $T\otimes\tau$ system will be prone to a trigonal distortion, whose magnitude in the weak to intermediate coupling case ($\alpha<1$) is only very weakly dependent on any deviation of the anharmonic coupling from the supersymmetric value. Likewise, our supersymmetric $E\otimes\varepsilon$ system has a warping term H_a which destroys the O(2) symmetry of the system under purely linear coupling, and whose magnitude affects tunnelling etc. In a practical situation quadratic coupling will vie with anharmonicity in determining e.g. the nature of the $E\otimes\varepsilon$ warping (equation (11.32) of Bates (1978)). As noted above, quadratic coupling can readily be included in a supersymmetric Hamiltonian and is not constrained by supersymmetry to the magnitude of cubic anharmonicity.

In each system, then, it is difficult to untangle the effects of the anharmonic term and the quadratic coupling term from experiment, and so to investigate whether a Jahn–Teller system is approximately supersymmetric. Certainly the constraints imposed by supersymmetry have as much realism as those associated with conventional higher symmetries of Jahn–Teller systems.

4. Supergroups and classifications of states

4.1. Group chains

In the absence of interactions the Hamiltonian H_N of equation (4) is invariant under the supersymmetry transformations generated by $S_j^i = f_i^+ b_j$ and $S_j^{i+} = f_i b_j^+$, $i, j = 1, 2, \ldots, N$. Together with $b_i^+ b_j$ and $f_i^+ f_j$ these generators close on the $(2N)^2$-dimensional supergroup $U(N/N)$ (see e.g. Freund and Kaplansky 1976).

In the interacting case, it is the subgroup $U(1/1)$ generated by S_N (equation (5)), S_N^+, H_N and fermion number $F = \Sigma_{i=1}^N f_i^+ f_i$ which is exact, since after replacing b_i by β_i (equation (11)) the algebraic construction is identical to that in the non-interacting case.

These considerations suggest that the eigenstates should be classified according to the group chain

$$U(N/N) \supset U(1/1) \otimes U(N) \supset U(1/1) \otimes O(N) \supset U(1) \otimes U(1) \otimes G, \tag{27}$$

the embedding of the ion point group G in $O(N)$ being defined by the fundamental branching rule $[1] \downarrow R$ where $R = E$ or T is the N-dimensional irrep of G under consideration. The final branching $U(1/1) \supset U(1) \otimes U(1)$ corresponds to the separation into boson and fermion subspaces.

In the non-interacting case the eigenstates are enumerated by the set

$$|B_1 B_2 \ldots B_N F_1 F_2 \ldots F_N\rangle \equiv \frac{(b_1^+)^{B_1} \ldots (b_N^+)^{B_N} (f_1^+)^{F_1} \ldots (f_N^+)^{F_N} |0\rangle}{\sqrt{(B_1! \ldots B_N!)}}. \tag{28}$$

An alternative group chain is suggested by these basis states:

$$U(N/N) \supset U(N) \otimes U(N) \supset \underbrace{(U(1) \otimes \ldots \otimes U(1))}_{N} \otimes \underbrace{(U(1) \otimes \ldots \otimes U(1))}_{N} \tag{29}$$

with separate factors for bosons (phonons) and fermions (ionic states). It is with respect to the $U(1/1) \otimes G$ basis that the classification is maintained in the presence of interactions.

In either case at the occupation number n level, an irreducible multiplet of $U(N/N)$ is labelled as $\{n\}$, corresponding to a rank-n graded-symmetric tensor (antisymmetrisations being required for fermionic tensor components). The supergroup branchings may be deduced from the general rule for $U(rt + su/ru + st) \supset U(r/s) \otimes U(t/u)$ (Dondi and Jarvis 1981, King 1975, 1982)

$$\{\lambda\} \downarrow \sum_{\zeta} \{\lambda\} \circ \{\zeta\} \times \{\zeta\} \tag{30}$$

where the symbol $\circ$ denotes an inner Kronecker product and the summation is over partitions λ in the symmetric group $S_{|\lambda|}$.

In the chain $U(N/N) \supset U(1/1) \otimes U(N)$ (equation (27)), we have

$$\{n\} \downarrow \{n\} \times \{n\} + \{n-1, 1\} \times \{n-1, 1\} + \ldots + \{n-N+1, 1^{N-1}\} \times \{n-N+1, 1^{N-1}\}, \tag{31}$$

using $(n) \circ (\zeta) = (\zeta)$, and that diagrams for $U(r/s)$ vanish unless they lie within an L-shaped envelope with horizontal and vertical arms of width r and s respectively. (For $U(1/1)$, this limits us to diagrams of one hook, and for $U(r) \cong U(r/0)$, to diagrams

with the number of rows less than or equal to r.) Finally, using the rule for $U(r/s) \supset U(r) \times U(s)$ (Dondi and Jarvis 1981, King 1975)

$$\{\lambda\}\downarrow \sum_{\text{all}\,\zeta} \{\lambda/\zeta\}\{\tilde{\zeta}\}, \tag{32}$$

we have in the present case simply

$$\{p, 1^q\}\downarrow \{p\}\{q\} + \{p-1\}\{q+1\}. \tag{33}$$

The branching rules of (32), (33) suffice to determine the phonon and ion content at level n of all irreps of G contained within a fixed irrep $\{n-k, 1^k\}$ of $U(N), 0 \leq k \leq N$.

In the chain $U(N/N) \supset U(N) \otimes U(N)$ (equation (27)) we have instead

$$\{n\}\downarrow \{n\}\times\{0\} + \{n-1\}\times\{1\} + \ldots + \{n-N\}\times\{1^N\}$$

with truncation if $n < N$.

The branchings $U(N) \supset O(N)$, known from classical group techniques, are

$N = 2$:

$$\{n\}\downarrow [n] + [n-2] + \ldots + ([0] \text{ or } [1]),$$
$$\{n-1, 1\}\downarrow [n-2] + [n-4] + \ldots + ([\tilde{0}] \text{ or } [1]);$$

$N = 3$:

$$\{n\}\downarrow [n] + [n-2] + \ldots + ([0] \text{ or } [1]),$$
$$\{n-1, 1\}\downarrow [\widetilde{n-1}] + [n-2] + [\widetilde{n-3}] + \ldots + ([\tilde{1}] \text{ or } [1]),$$
$$\{n-2, 1^2\}\downarrow [\widetilde{n-3}] + [\widetilde{n-5}] + \ldots + ([\tilde{1}] \text{ or } [\tilde{0}]).$$

Here $[p]$ has parity $(-1)^p$ and $[\tilde{p}]$ has opposite parity. The bracketed alternatives are for n even and n odd respectively.

The unperturbed Hamiltonian H_N has both $U(N)$ and $O(N)$ as invariance groups (for bosons or fermions or both). This means that the unperturbed eigenstates listed in the following tables may be classified irreducibly under these groups; this in turn suffices to find these states and to give a full parentage classification for the entries listed, the perturbed eigenstates being in one-one correspondence.

The spatial symmetry group of the true eigenstates is the octahedral group O in our examples. The embedding of O in $O(N)$, $N = 2, 3$, is defined by taking the N one-particle states in either the boson or fermion space as partners of the vector representation of $O(N)$. This implies an embedding $O(N) \supset O$ which has no necessary connection with the embedding of an octahedron in physical N-dimensional space. (In fact O(2) does not even contain O as a subgroup.) This distinction, together with the branching rules for the embeddings we require are discussed by Butler (1981) (see his equations (7.4.1), (7.4.2)).

4.2. $E \otimes \varepsilon$

We list in table 1 representative eigenfunctions for each of the lowest levels of the supersymmetric $E \otimes \varepsilon$ system, in the notation of equation (28) with $N = 2$ and with the omission of overall normalisation factors and of terms of order α. The other members of each level may be obtained by applying supersymmetry or octahedral

Table 1. Supersymmetric states and energies for the E⊗ε problem†.

Type	Representative state	Unperturbed energy	Degeneracy	Energy shift	Classification $U(2/2) \supset U(1/1) \otimes O(2) \supset U_1 \otimes U_1 \otimes O$					
a	$\|0000\rangle$	0	1	0	{0}	{0}	{0}	0	0	0
a	$\|1000\rangle$	1	4	−32	{1}	{1}	{1}	1	0	2
								0	1	
a	$\|1100\rangle$	2	4	−32	{2}	{2}	{2}	2	0	2
								1	1	
a	$\|2000\rangle + \|0200\rangle$	2	2	−192	{2}	{2}	{0}	2	0	0
								1	1	
b	$\|0011\rangle$	2	2	0	{2}	{1, 1}	{$\tilde{0}$}	1	1	$\tilde{0}$
								0	2	
a	$\|3000\rangle - \sqrt{3}\|1200\rangle$	3	2	0	{3}	{3}	{3}	3	0	0
								2	1	
a	$\sqrt{3}\|2100\rangle - \|0300\rangle$	3	2	0	{3}	{3}	{3}	3	0	$\tilde{0}$
								2	1	
b	$\|0111\rangle$	3	4	−32	{3}	{2, 1}	{1}	2	1	2
								1	2	
a	$\sqrt{3}\|3000\rangle + \|1200\rangle$	3	4	−320	{3}	{3}	{1}	3	0	2
								2	1	
a	$\sqrt{3}(\|4000\rangle + \|0400\rangle) + \sqrt{2}\|2200\rangle$	4	2	−576	{4}	{4}	{0}	4	0	0
								3	1	
b	$\|2011\rangle + \|0211\rangle$	4	2	−192	{4}	{3, 1}	{$\tilde{0}$}	3	1	$\tilde{0}$
								2	2	
a	$\|4000\rangle - \|0400\rangle$	4	4	−416	{4}	{4}	{2}	4	0	2
								3	1	
a	$\|3100\rangle - \|1300\rangle$	4	4	+64	{4}	{4}	{4}	4	0	2
								3	1	
b	$\|1111\rangle$	4	4	−32	{4}	{3, 1}	{2}	3	1	2
								2	2	

† Overall normalisations are omitted. Energy shifts are in units of α^2. The 'type' label is defined in § 5.2.3.

operations. For example, corresponding to $|1\ 1\ 0\ 0\rangle$ we have

$$S^+|1\ 1\ 0\ 0\rangle = (f_1^+ b_1 + f_2^+ b_2) b_1^+ b_2^+ |0\rangle = |1\ 0\ 0\ 1\rangle + |0\ 1\ 1\ 0\rangle,$$

while octahedral operations mix in $|2\ 0\ 0\ 0\rangle - |0\ 2\ 0\ 0\rangle$ and $|1\ 0\ 1\ 0\rangle - |0\ 1\ 0\ 1\rangle$ respectively.

The classification of these levels in each group chain is also given. The embedding of O in O(2) (see § 4.1) is defined by the rule $[1]\downarrow E(2)$ (numerical irrep labels for O are those of Butler (1981)), together with the effects of taking symmetrised products. The resulting branching rules are $[0]\downarrow A_1(0)$, $[\tilde{0}]\downarrow A_2(\tilde{0})$, $[3p]\downarrow A_1 + A_2\ (0+\tilde{0})$, $[3p \pm 1]\downarrow E(2)$ where p is an integer.

The complete branching $U(2/2) \supset U(1/1) \otimes O$ becomes

$$\{3p\}\downarrow \mathbf{2} \times (2pE + p(A_1 + A_2)), \qquad p > 0,$$

$$\{3p \pm 1\}\downarrow \mathbf{2} \times ((2p \pm 1)E + p(A_1 + A_2)),$$

where the U(1/1) doublets **2** are of the form $\{3p\}$ or $\{3p-1, 1\}$. The precise sharing of octahedral irreps between these forms depends on n (mod 6).

In some cases it is necessary to use the O(2) parentage label or the U(1) boson or fermion content, to distinguish levels. (For example the octahedral doublet containing $|3\ 1\ 0\ 0\rangle - |1\ 3\ 0\ 0\rangle$ is unchanged under the operation $b_1 \to b_2$, $b_2 \to -b_1$; its character, 2, agreeing with that of [4] of O(2).)

As in § 2, it is possible to calculate the perturbed energy of these states up to say second order in α. These energy shifts are listed in table 1 and depicted in figure 1. For a state of the form $|B_1 B_2 F_1 F_2\rangle$ this energy shift is given by

$$\Delta E = \alpha^2(-32H_{12} + 48(F_1 - F_2)(B_2 - B_1) - 24(B_1^2 + B_2^2) + 32B_1B_2 - 8(B_1 + B_2)),$$

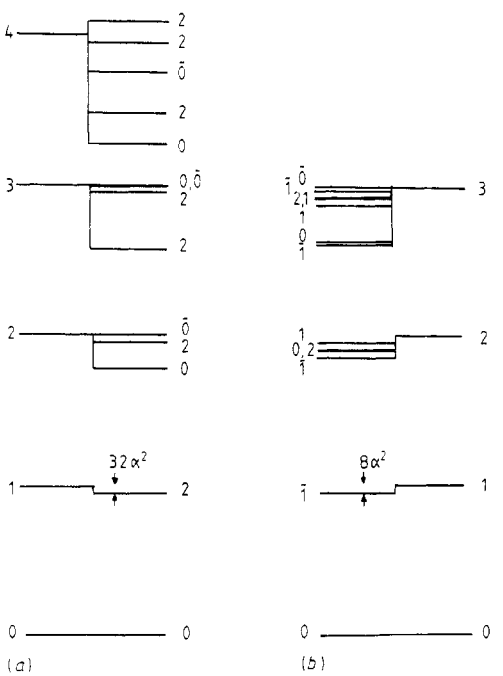

Figure 1. Energy level schemes for (*a*) the $E \otimes \varepsilon$ and (*b*) $T \otimes \tau$ supersymmetric Jahn–Teller Hamiltonians.

where $H_{ij} = 1$ if $F_i \neq F_j$, and $H_{ij} = 0$ otherwise.

The ground state is of necessity unshifted; it is curious that just one of the remaining shifts is positive.

4.3. $T_2 \otimes \tau_2$

We list in table 2 representative eigenfunctions, classification labels and second-order energy shifts for each level as for $E \otimes \varepsilon$ in § 4.2. Energy shifts are depicted in figure 1.

The embedding of O in O(3) (see § 4.1) is defined by the rule $[1] \downarrow T_2(\tilde{1})$ (note the parity, despite the positive spatial parity of the physical states) together with symmetrised products. This gives $[0] \downarrow A_1(0)$, $[\tilde{0}] \downarrow A_2(\tilde{0})$, $[\tilde{1}] \downarrow T_1(1)$, $[2] \downarrow E + T_2(2+\tilde{1})$, $[\tilde{2}] \downarrow E + T_1(2+1)$, $[\tilde{3}] \downarrow 0 + 1 + \tilde{1}$, $[3] \downarrow \tilde{0} + 1 + \tilde{1}$, etc.

A state of the form $|B_1 B_2 B_3 F_1 F_2 F_3\rangle$ has the energy shift

$$\Delta E = -4\alpha^2(H_{12} + H_{23} + H_{31} + 2(B_1 + B_2 + B_3) + 2(B_1 B_2 + B_2 B_3 + B_3 B_1)).$$

Similar results will hold for the $T_1 \otimes \tau_2$ system, although the change of parities in the branchings $O(3) \supset O$ complicate some assignments.

4.4. Supersymmetry and physics: energies

As indicated in tables 1 and 2, certain vibrational states (those in which the U(1) fermion content is zero) have energies which are constrained by supersymmetry to equal those of corresponding states with one fermion state occupied (i.e. with a Jahn–Teller active level occupied) and one less quantum of vibration. While the supersymmetric Hamiltonian includes the Jahn–Teller coupling H_c, the effects of this term will vanish in states with no fermions present. For purely vibrational states, then, the energy shifts are to be attributed entirely to anharmonicity (H_a). Supersymmetry relates these energy shifts to those induced by the Jahn–Teller coupling together with anharmonicity in a different system (one incorporating a Jahn–Teller active state).

No such simple physical interpretation is apparent in the cases where multifermion states are present. Two Jahn–Teller active ions would not answer the requirements of the Pauli exclusion principle in the formalism of this paper.

5. Dressing factors

In this section we are concerned with higher-order corrections of some basic interaction vertex. In condensed matter theory these would often be called renormalisation effects; a relativistic field theorist might prefer the description of radiative dressing.

5.1. Ham reduction factors for Jahn–Teller ions

A purely electronic interaction acting within a Jahn–Teller active level will have its matrix elements reduced by the effect of the coupling H_c to vibrations and in addition of the anharmonicity H_a of the vibrations. The amount of the reduction is of course characteristic of the various interactions, but depends on the choice of electronic operator $O^{\mu m}$ only through its point group symmetry label μ, independently of its physical origin or component m within the irrep μ; we write the associated reduction factor as $K_\lambda(\mu)$, $\lambda = 2\,(\tilde{1})$ denoting $E \otimes \varepsilon$ $(T \otimes \tau)$.

Table 2. Supersymmetric states and energies for $T_2 \otimes \tau_2$.

Type	Representative state	Unperturbed energy	Degeneracy	Energy shift	Classification $U(3/3) \supset U(1/1) \otimes O(3) \supset U_1 \otimes U_1 \otimes O$					
a	$\|000000\rangle$	0	1	0	{0}	{0}	[0]	0	0	0
a	$\|100000\rangle$	1	6	−8	{1}	{1}	[1]	1 0	0 1	$\tilde{1}$
a	$\|200000\rangle + \|020000\rangle + \|002000\rangle$	2	2	−16	{2}	{2}	[0]	2 1	0 1	0
a	$\|200000\rangle - \|020000\rangle$	2	4	−16	{2}	{2}	[2]	2 1	0 1	2
b	$\|000011\rangle$	2	6	−8	{2}	{1, 1}	$[\tilde{1}]$	1 0	1 2	1
a	$\|011000\rangle$	2	6	−24	{2}	{2}	[2]	2 1	0 1	$\tilde{1}$
a	$\|111000\rangle$	3	2	−72	{3}	{3}	[3]	3 2	0 1	0
c	$\|000111\rangle$	3	2	0	{3}	$\{1, 1^2\}$	$[\tilde{0}]$	1 0	2 3	$\tilde{0}$
b	$\|100011\rangle - \|010101\rangle$	3	4	−16	{3}	{2, 1}	$[\tilde{2}]$	2 1	1 2	2
a	$\|120000\rangle - \|102000\rangle$	3	6	−24	{3}	{3}	[3]	3 2	0 1	1
b	$\|010110\rangle + \|001101\rangle$	3	6	−16	{3}	{2, 1}	$[\tilde{2}]$	2 1	1 2	1
a	$\|120000\rangle + \|102000\rangle + \sqrt{3}\|300000\rangle$	3	6	−376/5	{3}	{3}	[1]	3 2	0 1	$\tilde{1}$
a	$\sqrt{3}(\|120000\rangle + \|102000\rangle) - 2\|3000000\rangle$	3	6	−24/5	{3}	{3}	[3]	3 2	0 1	$\tilde{1}$

When the conventional higher symmetries (§ 1) are present, the reduction factors often simplify. Since the supersymmetric Hamiltonians are highly constrained, the associated reduction factors are well defined (depending only on the one parameter α of § 3.2). For these reasons, it is of intrinsic interest to compute these reduction factors. The formalism of Payne and Stedman (1983a) is ideally suited to this task, since anharmonic effects are included systematically.

In carrying out their method to fourth order, we have to compute the diagrams of figure 2(a)–(g). Figure 2(a) is the standard second-order term from H_c, and figure 2(b)–(e) the corresponding terms at fourth order. These are evaluated in Payne and Stedman (1983b). Cubic anharmonicity contributes a fourth-order contribution as in figure 2(f), and quartic anharmonicity contributes figure 2(g). In addition, fourth-

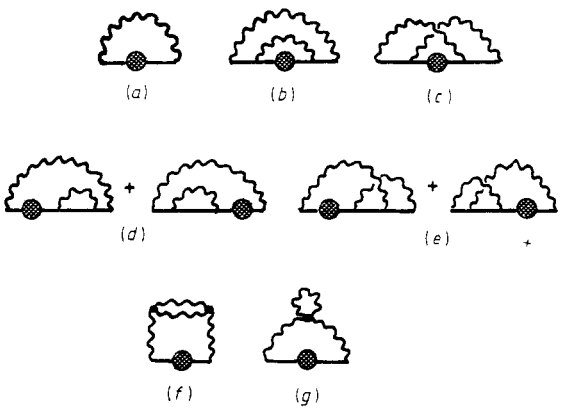

Figure 2. Diagrams contributing to reduction factors at fourth order.

order corrections to the denominators appearing in figure 2(a) are required. The result (see appendix) is

$$K_\lambda(\mu) = 1-(2n+1)r_\lambda^\mu\alpha^2-(n^2+n)s_\lambda^\mu\alpha^4+t_\lambda^\mu\alpha^4 \tag{34}$$

with the coefficients given in table 3; n is the Bose–Einstein factor.

These reduction factors obey the standard sum rules

$$K_2(2)=\tfrac{1}{2}(1+K_2(\tilde{0})), \qquad 2(K_{\tilde{1}}(2)-1)=3(K_{\tilde{1}}(1)-K_{\tilde{1}}(\tilde{1})), \tag{35}$$

which are associated with time-reversal considerations, and are applicable at fourth order in models with one vibrational frequency (Payne and Stedman 1983c). However, they show no obvious new special feature, to be associated with supersymmetry *per se*. For that we must enlarge the concept of a reduction factor (§ 5.2).

5.2. Supersymmetry and physics: reduction factors for vibrational operators

5.2.1. Introduction. Supersymmetry requires a connection between the properties of a Jahn–Teller ion and those of the anharmonic vibrations with which it is (supersymmetrically) coupled. In the case of the reduction factors just calculated, we expect to find comparable reduction factors for similar vibrational operators.

In order to quantify this, consider first as in § 5.1 a purely electronic irreducible tensor operator $O^{\mu m}$, μ being the irrep and m the component label under the point

Table 3. Coefficients in the expansion of (34) for the reduction factor $K_\lambda(\mu)$. $\lambda = 2\,(\tilde{1})$ applies to $E \otimes \varepsilon$ $(T \otimes \tau)$.

λ	μ	r_λ^μ	s_λ^μ	t_λ^μ
2	$\tilde{0}$	64	$2^{12}\times 7/3$	$2^8\times 73/9$
2	2	32	$2^{11}\times 7/3$	$2^7\times 73/9$
$\tilde{1}$	2	12	$2^3\times 3^3/13$	$-2^2\times 3\times 47$
$\tilde{1}$	1	12	$2^3\times 353$	$-2^2\times 11\times 13$
$\tilde{1}$	$\tilde{1}$	4	$2^3\times 7\times 17$	$-2^2\times 7^2$

group G. If this is expanded in terms of fermion creation and annihilation operators, themselves also irreducible tensor operators with irrep λ (E or T in the octahedral examples discussed here),

$$O^{\mu m} = \sum_{ij} O_{ij}^{\mu m} f_i^+ f_j \tag{36}$$

the coefficients are proportional to Clebsch–Gordan symbols of G by the Wigner–Eckart theorem, and we may write in coupled-tensor notation

$$O^{\mu m} = [f^{+\lambda} f^\lambda]_m^\mu. \tag{37}$$

5.2.2. Zero temperature. Even under perturbation, the vacuum state may be ignored; no fermion operator, and only symmetric boson operators, can give any matrix element in it. The lowest states of interest are then the one-particle states.

We write one-fermion zero-boson eigenstates of H_N as $|\phi_l\rangle_0 = f_l^+|0\rangle$ (i.e. $F_i = \delta_{il}$, $B_i = 0$), and the corresponding eigenstates of the supersymmetric Hamiltonian as $|\phi_l\rangle$. At low temperatures, these will give the leading contributions to all expectation values.

The Jahn–Teller reduction factor relates the matrix elements of $O^{\mu m}$ in these two sets of states (i.e. for the interacting and for the non-interacting case):

$$\langle\phi_l|O^{\mu m}|\phi_{l'}\rangle = K_\lambda(\mu)\,{}_0\langle\phi_l|O^{\mu m}|\phi_{l'}\rangle_0. \tag{38}$$

Since the states $\{|\phi_l\rangle\}$ are normalised eigenstates of H_1 with eigenvalue E say, we may write (using $H = (S+S^+)^2$):

$$\langle\phi_l|O^{\mu m}|\phi_{l'}\rangle = E^{-2}\langle\phi_l|(S+S^+)^2 O^{\mu m}(S+S^+)^2|\phi_{l'}\rangle. \tag{39}$$

The state $|\psi_l\rangle \equiv E^{-1/2}(S+S^+)|\phi_l\rangle$ is the bosonic counterpart of $|\phi_l\rangle$ ($|\psi_l\rangle_0 = b_l^+|0\rangle$), and is normalised by the $E^{-1/2}$ factor (supersymmetry makes $|\psi_l\rangle$ and $|\phi_l\rangle$ degenerate). Hence

$$\langle\phi_l|O^{\mu m}|\phi_{l'}\rangle = E^{-1}\langle\psi_l|\bar{O}^{\mu m}|\psi_{l'}\rangle \tag{40}$$

where

$$\bar{O}^{\mu m} \equiv (S+S^+)O^{\mu m}(S+S^+). \tag{41}$$

The commutation relations of equations (10), (12) etc enable us to commute $O^{\mu m}$ through $(S+S^+)$ etc, so as to write $\bar{O}^{\mu m} = \Sigma_{ij} O_{ij}^{\mu m}\beta_i^+\beta_j + \underline{x}$ where the terms in $\underline{x}$ have either a leading fermion creation operator or a trailing fermion annihilation operator. Since even under perturbation the states $\{|\psi_l\rangle\}$ will not contain any fermion creation

operators, $\underline{x}$ will not contribute to the matrix element, and we conclude that

$$\bar{O}^{\mu m} \equiv [\beta^{+\lambda}\beta^{\lambda}]^{\mu}_{m}. \tag{42}$$

Equations (40), (42) indicate a link between the effects of the perturbation interactions on matrix elements of bosonic operators in bosonic states, and similar effects on matrix elements for fermions. The link is not a direct analogy for two reasons; a factor E^{-1}, containing perturbative corrections, appears in equation (40), and $\bar{O}^{\mu m}$ differs from the more obvious analogue

$$P^{\mu m} = [b^{+\lambda}b^{\lambda}]^{\mu}_{m}. \tag{43}$$

An external coupling to the vibrational system, such as external stress, will naturally be expanded in terms of the fundamental operators b_l, b_l^+ and thus of the operators $P^{\mu m}$. A natural definition of vibrational, as opposed to electronic, reduction factor, $L_\lambda(\mu)$ is thus given (in analogy with equation (38)) by

$$\langle\psi_l|P^{\mu m}|\psi_{l'}\rangle = L_\lambda(\mu)\ {}_0\langle\psi_l|P^{\mu m}|\psi_{l'}\rangle_0. \tag{44}$$

The $L_\lambda(\mu)$ would then parametrise the effects of anharmonicity on the matrix elements associated with the external coupling. (The analogy is not complete in that $L_\lambda(0)$ is not necessarily unity.) If we combine equation (40), the corresponding equation when $\alpha = 0$ (when $\bar{O}^{\mu m} = P^{\mu m}$), equations (38), (44) and the result

$$\langle\psi_l|\bar{O}^{\mu m}|\psi_{l'}\rangle = c_\lambda(\mu)\langle\psi_l|P^{\mu m}|\psi_{l'}\rangle \tag{45}$$

given by the Wigner–Eckart theorem, we obtain

$$L_\lambda(\mu) = EK_\lambda(\mu)/(E_0 c_\lambda(\mu)) \tag{46}$$

where E_0 is the unperturbed energy. Equation (46) quantifies the restriction imposed by supersymmetry on the electronic (Ham) and vibrational reduction factors.

We have used perturbation theory to determine all wavefunctions and operators in these expressions and thus have evaluated all the terms in (46) explicitly to second order (table 4). It follows that, for example, $L_2(2) = K_2(2)$, i.e. the electronic and the vibrational reduction factors are equal in this case.

While these results relate closely to observables, we cannot suggest a method of determining vibrational dressing factors purely from experiment. They might rather

Table 4. Electronic and vibrational reduction factors for several supersymmetric octahedral Jahn–Teller systems to second order and at zero temperature. The labels 0, $\tilde{0}$, 2, 1, $\tilde{1}$ denote A_1, A_2, E, T_1, T_2 irreps; the supersymmetric one-quantum energies are $E(\lambda = 2) = 1 - 32\alpha^2$ (table 1), $E(\lambda = \tilde{1}) = 1 - 8\alpha^2$ (table 2); the constants O_{ij}^{00} are chosen to be the unnormalised values δ_{ij}, so that $\bar{O}^{00}$ is just the vibrational part of the supersymmetric Hamiltonian (equation (15)).

λ	μ	$K_\lambda(\mu)$	$L_\lambda(\mu)$	$c_\lambda(\mu)$
2	0	1	$1+56\alpha^2$	$1-88\alpha^2$
2	$\tilde{0}$	$1-64\alpha^2$	$1-96\alpha^2$	1
2	2	$1-32\alpha^2$	$1-32\alpha^2$	$1-32\alpha^2$
$\tilde{1}$	0	1	$1+15\alpha^2$	$1-23\alpha^2$
$\tilde{1}$	2	$1-12\alpha^2$	$1-18\alpha^2$	$1-2\alpha^2$
$\tilde{1}$	1	$1-12\alpha^2$	$1-16\alpha^2$	$1-4\alpha^2$
$\tilde{1}$	$\tilde{1}$	$1-4\alpha^2$	$1+2\alpha^2$	$1-14\alpha^2$

be derived from a comparison of the observed matrix elements of a lattice operator such as stress with the predictions of a harmonic model. Methods of determining Ham reduction factors experimentally are well documented (Bates 1978, Challis and de Göer 1983). In principle, the measurement of such factors, together with a comparison with table 4, would give one estimate of the degree to which a particular system approximated the supersymmetric case.

5.2.3. Finite temperature. The states $\{2\}, \{3\} \ldots$ of $U(N/N)$ will affect the reduction factors at higher temperature. The electronic reduction factors may be defined through the thermal expectation values of the operators (Payne and Stedman 1983a) and indeed thermal factors are included in the explicit calculation of § 5.1. The question arises as to how far the isomorphisms of § 5.2.2 can be generalised to cover these effects.

The eigenstates of the full Hamiltonian may be classified into (a) the vacuum state, and also those in which the supersymmetry renders degenerate two states with fermion numbers one and zero; (b) a similar pair with fermion numbers two and one; (c) a pair with fermion numbers higher than one. The supersymmetry operation always links states with fermion numbers differing by unity, and never of itself produces triplets or quartets (since $S^2 = 0$). This classification is indicated in tables 1 and 2.

The argument of § 5.2.2 may be generalised formally to states of type (a) only; within the bosonic partners of these states, the matrix elements of $\underline{x}$ may be ignored as before. The connection between the types of reduction factor is rather less close; if we define $K_\lambda(\mu, T)$ at finite temperature by

$$\sum_{l\in a} \exp(-\beta E_l)\langle\phi_l|O^{\mu m}|\phi_{l'}\rangle \Big/ \sum_{l\in a} \exp(-\beta E_l)$$
$$= K_\lambda(\mu, T) \sum_{l\in a} \exp(-\beta E_l^0)_0\langle\phi_l|O^{\mu m}|\phi_{l'}\rangle_0 \Big/ \sum_{l\in a} \exp(-\beta E_l^0)$$

in which $|\phi_l\rangle$ is summed over all possible one-fermion states of type (a), then the energy factor in (40) gives a weighted sum different from the thermal average required for the analogous vibrational reduction factor. Together with the special problems of states of type (b) and (c) (when equation (42) is inapplicable, although we note that type (a) states are the most numerous) this makes the correspondence between electronic and vibrational reduction factors less direct in the finite-temperature case.

5.3. Field theoretic consequences

Finally, we comment on the graphical consequences of supersymmetry for such field theoretic diagrams as those computed in § 5.1. The method of calculation developed in Payne and Stedman (1983a) (appendix 1) requires the invariance of each vertex independently under the point group; this allows the (graphical) breakdown of any diagram into group invariants and *nj* symbols. This cannot be repeated directly for supersymmetry, since supergroup operators mix different vertices (e.g. the third degree vertex for two fermions and one boson, with that for three bosons). Supersymmetric actions have of course been given by Salam and Strathdee (1975) and Cooper and Freedman (1983); however, a canonical analysis expressing the Hamiltonian in terms of superfields would permit a supergraph analysis of this problem. In this, a supervertex would integrate the above vertices into a single entity which was invariant under the supergroup. We might then expect to generalise the graphical analysis of symmetry constraints used by Payne and Stedman (1983a) in Jahn–Teller systems to a graphical analysis of supersymmetry.

Acknowledgment

We thank Professor B G Wybourne for the encouragement that made this collaboration possible.

Appendix. Calculation of electronic reduction factors for the supersymmetric case

In the method of Payne and Stedman (1983a) an intermediate set of parameters $d(\mu)$ are found. These in turn are linear combinations of a symmetry-dependent factor J_i^μ corresponding to the *nj* symbols appearing in figure 2(*i*) and of an energy-dependent factor X_i.

The diagrams of figure 2(*a*), (*f*) and (*g*) have the same structure, and thus the same J^μ factors; their joint contribution to fourth order is (including fourth-order corrections to the denominators of figure 2(*a*))

$$d(\mu) = J_a^\mu[(2n+1)\gamma - 2\gamma^2 + (\gamma_3/9)(114n^2+114n+29) - 3\gamma_4(2n+1)^2]$$

where $\gamma \equiv g/\omega^2$, $\gamma_3 \equiv \tilde{g}_3/\omega^4$, $\gamma \equiv \tilde{g}_4/\omega^3$, ω is an overall frequency factor scaling the supersymmetric Hamiltonian, $n = (\exp(\beta\omega)-1)^{-1}$, $\beta = 1/kT$. The reduced matrix elements (in the notation of Payne and Stedman (1983b)) have the values

$$g = |\lambda|^{-1} \sum_{ijp} |V_{ijp}|^2,$$

$$\tilde{g}_3 = |\lambda|^{-1} \sum_{ijpkl} |V_{ijp}|^2 |W_{pkl}|^2, \qquad \tilde{g}_4 = |\lambda|^{-1} \sum_{ijpkl} |V_{ijp}|^2 W_{ppkl}.$$

When the interaction constants $V_{ipk\ldots}$, $W_{klm\ldots}$ appearing in (22) and (24) are inserted, we obtain the parameters of table A1.

Table A1. Reduced matrix elements for the supersymmetric Hamiltonians.

	E⊗ε	T⊗τ
γ	$32\alpha^2$	$8\alpha^2$
γ_3	$448\alpha^4$	$144\alpha^4$
γ_4	$96\alpha^4$	$16\alpha^4$

The fourth-order diagrams of figure 2(*i*), $i = b$ to e contribute

$$d(\mu) = \sum_i J_i^\mu X_i \tag{38}$$

with $4X_b = 4X_c = X_d = X_e = (2n^2+2n+1)\gamma^2$, and, the J_i^μ values required are given in Payne and Stedman (1983b, c) and are summarised in table A2. The reduction factors are given by

$$K_\lambda(\mu) = 1 + [d(\mu) - d(0)][1 - d(0)].$$

Upon insertion of the tabulated parameters into these equations, we derive (34).

Table A2. Contributions from linear coupling at fourth order, to the *nj* symbol content J_λ^μ of figure 2(*i*)'s contribution to the factor $d(\mu)$. $\lambda = 2\ (\tilde{1})$ corresponds to $E \otimes \varepsilon$ $(T \otimes \tau)$.

		i	*a*	*b*	*c*	*d*	*e*
λ	μ						
2	0		1	1	—	2	—
2	$\tilde{0}$		−1	1	—	−2	—
2	2		—	—	1	—	—
$\tilde{1}$	0		1	1	$\frac{1}{2}$	1	$\frac{1}{2}$
$\tilde{1}$	2		$-\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{4}$
$\tilde{1}$	1		$-\frac{1}{2}$	$\frac{1}{4}$	—	$-\frac{1}{2}$	$-\frac{1}{4}$
$\tilde{1}$	$\tilde{1}$		$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{4}$

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