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Algebraic approach to nuclear quasimolecular spectra

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It is suggested that nuclear quasimolecular spectra are dominated by dipole rather than quadrupole degrees of freedom. An algebraic approach to these dipole modes in terms of the group U(4) is proposed. One of the dynamical symmetries of the corresponding algebraic structure, O(4), is discussed and shown to yield spectra of molecular rotation-vibration type.

[NUCLEAR REACTIONS Quasimolecular spectra, algebraic approach, O(4) symmetry.]

After the discovery[1] of isolated, narrow, resonances in heavy-ion scattering around the Coulomb barrier, several attempts have been made in order to provide a quantitative description of their observed properties. These attempts are based on the extrapolation of ideas and techniques used in the description of the low-lying collective nuclear states. Since these states are dominated by quadrupole degrees of freedom, most interpretations suggest either the occurrence of quadrupole rotation-vibration spectra,[2] or of quadrupole excitations of the ions.[3,4] Although these approaches describe qualitatively the observed features, no quantitative agreement with experiment has yet been achieved.

In this Communication, I wish to point out that, if molecular states are formed in the collision, it is more likely that their structure is similar to that observed in diatomic molecules, rather than being similar to that of low-lying nuclear states. In particular, since it is well known that rotation-vibration spectra of diatomic molecules are dominated by *dipole* degrees of freedom[5] (the fundamental quantity here being the vector $\vec{R}$ representing the distance between the two atoms), one may expect that quasimolecular states in heavy-ion collisions are also dominated by dipole, rather than quadrupole, degrees of freedom.

A quantitative study of nuclear quasimolecular spectra should then be done as in the case of molecular spectra. States of diatomic molecules are characterized by two quantum numbers, a vibrational quantum number, v, and the angular momentum L. A purely empirical description of the energy levels is given by the Dunham expansion[6]

$$E(v,L)=\sum_{ij} Y_{ij}(v+\tfrac{1}{2})^i[L(L+1)]^j \ . \tag{1}$$

Here, the coefficients Y_{ij} are determined from experiment and provide information on the moment of inertia and on the vibrational frequency of the molecule. However, since the rotation-vibration bands in (1) have no cutoff, it is not possible to extract information on the molecular dissociation energy and thus on the configurations responsible for the binding. A more fundamental description of the energy levels is obtained by constructing an interatomic (in the present case internuclear) potential $V(R)$, and solving the corresponding Schrödinger equation. Since $V(R)$ is unknown, one usually expands it into a set of known functions with arbitrary coefficients to be determined from experiment. In the molecular case, the functions are usually polynomials in R,[7]

$$V(R)=\sum_n a_n\left(\frac{R-c}{b}\right)^n \ . \tag{2}$$

To adjust the coefficients a_n is a rather complex and time consuming problem. In this Communication, I would like to propose an alternative, algebraic, approach which is on one side relatively simple and on the other side very detailed. This approach is based on the realization that rotation-vibration spectra in r

dimensions can be constructed using the Lie algebra of the unitary groups in $r+1$ dimensions.[8] Applications of these techniques to quadrupole ($r=5$) spectra have led to a very detailed description of low-lying collective states in nuclei.[9] Thus, it is likely that the application of these techniques to dipole ($r=3$) spectra may lead to a similar description of molecular and quasimolecular spectra.

For $r=3$, the appropriate group is U(4). In order to show explicitly that the algebraic approach leads to molecular rotation-vibration spectra, it is convenient to realize the algebra in terms of creation and annihilation operators. To this end, I introduce a set of four boson operators, divided into a scalar, $L=0$, operator, denoted by σ, and a vector, $L=1$, operator denoted by $\pi_\mu (\mu=0, \pm 1)$. These operators are assumed to have parity $(-)^L$. The introduction of the vector (π) boson reflects the dipole nature of the problem. In order to calculate energy spectra, I next expand the Hamiltonian, H, in terms of boson operators. If, for simplicity, one stops at quadratic terms, this yields

$$\begin{aligned} H = {} & \epsilon_\sigma(\sigma^\dagger \cdot \sigma) + \epsilon_\pi(\pi^\dagger \cdot \tilde{\pi}) + \sum_{L=0,2} \tfrac{1}{2}(2L+1)^{1/2} c_L [[\pi^\dagger \times \pi^\dagger]^{(L)} \times [\tilde{\pi} \times \tilde{\pi}]^{(L)}]^{(0)} \\ & + u_0 [[\sigma^\dagger \times \sigma^\dagger]^{(0)} \times [\sigma \times \sigma]^{(0)}]^{(0)} + u_2 [[\pi^\dagger \times \pi^\dagger]^{(0)} \times [\sigma \times \sigma]^{(0)} + [\sigma^\dagger \times \sigma^\dagger]^{(0)} \times [\tilde{\pi} \times \tilde{\pi}]^{(0)}]^{(0)} \\ & + u_1 [[\pi^\dagger \times \sigma^\dagger]^{(1)} \times [\tilde{\pi} \times \sigma]^{(1)}]^{(0)} \quad . \end{aligned} \tag{3}$$

Here $\tilde{\pi}_\mu = (-)^{1-\mu} \pi_{-\mu}$ and the square brackets denote tensor products. This expansion corresponds to the expansion of the potential $V(R)$ into a set of given functions, Eq. (2). Energy spectra are now obtained by diagonalizing H in the space $[N]$ of the totally symmetric irreducible representations of the group U(4) generated by the 16 bilinear products $G_{\alpha\alpha'} = b^\dagger_\alpha b_{\alpha'}$ ($\alpha = 1,2,3,4$; $b_\alpha \equiv s, \pi_\mu$). While the potential approach involves the solution of a differential equation, the algebraic approach involves the solution of a matrix equation and thus it is much simpler to deal with. A computer program to solve this problem has been written and it is available on request.[10] In addition, in the algebraic approach, it is possible to construct in a simple way analytic solutions to the eigenvalue problem. These simple cases correspond to dynamical symmetries of the Hamiltonian, and they can be found by performing a group theoretical analysis of (3) similar to that performed in the quadrupole case.[9] Here, there are only two dynamical symmetries, corresponding to the group chains (I) $\mathrm{U}(4) \supset \mathrm{O}(4) \supset \mathrm{O}(3) \supset \mathrm{O}(2)$ and (II) $\mathrm{U}(4) \supset \mathrm{U}(3) \supset \mathrm{O}(3) \supset \mathrm{O}(2)$. For the purpose of displaying the nature of the spectrum, I will explicitly construct the solution corresponding to the symmetry (I). In this case, the following quantum numbers, in addition to N, classify uniquely the states: a quantum number, ω, which characterizes the representations of O(4), $\omega = N, N-2, \dots, 1$ or 0 (N is odd or even); the angular momentum, L, and its projection, M; the values of L contained in each O(4) representation, ω, are $L=0,1,\dots,\omega$. Using techniques similar to those discussed in Ref. 9, one can find the most general solution corresponding to this symmetry type

$$E(N,\omega,L,M) = A\tfrac{1}{4}(N-\omega)(N+\omega+2) + BL(L+1) \quad , \tag{4}$$

where A and B are arbitrary constants. The structure of the corresponding spectrum is shown in Fig. 1. One can see that this structure is that typical of a diatomic or dinuclear molecule.[5] To make the connection even more apparent, it is convenient to rewrite (4), by introducing a vibrational quantum number $v=(N-\omega)/2$, as

$$\begin{aligned} E(v,L) = {} & -A\frac{2N+3}{4} + A(N+2)(v+\tfrac{1}{2}) \\ & - A(v+\tfrac{1}{2})^2 + BL(L+1) \quad . \end{aligned} \tag{5}$$

Comparing (5) with (1) one sees that a dynamical O(4) symmetry corresponds to an empirical expansion with only three coefficients Y_{10}, Y_{20}, and Y_{01}, in addition to the overall constant, Y_{00}. Moreover, $Y_{10}/Y_{20} = -(N+2)$.

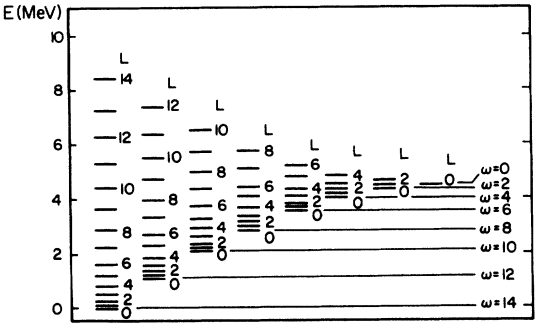

FIG. 1. Typical molecular spectrum with O(4) symmetry. The energy levels are given by Eq. (4) with $N=14$, $A=80$ keV and $B=40$ keV. The energy scale is that appropriate to nuclear molecular spectra. For homonuclear molecules the negative parity, $1^-, 3^-, \dots$ states are missing because of reflection symmetry (Ref. 5).

The discussion above has been confined to a treatment of molecular resonances as bound (or quasibound) states arising from one particular channel. Thus the states calculated in this way have no width and are not coupled to other channels. A detailed study of heavy-ion scattering shows that this is a complex multichannel problem. In $^{12}C-{}^{12}C$ scattering for example, at least the following channels should be included: (1) the elastic channel; (2) the inelastic channels in which ^{12}C is excited to the first few low-lying levels (2^+(4.44 MeV), 0^+(7.65 MeV), 3^-(9.64 MeV)); and (3) rearrangements channels such as $^{20}Ne+\alpha$, $^{16}O+{}^8Be$. The multichannel problem can be attacked in a potential approach by introducing diagonal, V_{ii}, and off-diagonal, V_{ij} $(j\neq i)$, potentials, and solving the appropriate coupled channel equations (here i denotes the channels). The same problem can be attacked in the algebraic approach by introducing an algebraic diagonal, H_{ii}, and off-diagonal, H_{ij}, Hamiltonian and solving the corresponding set of algebraic equations. The virtue of the algebraic approach is that matrix equations are relatively more easy to solve than differential equations. One possible way in which this program can be carried out in practice is to assign to the boson operators an additional, internal, quantum number, $i=1,\ldots,n$, which labels the various channels. The corresponding operators become now an array, $b_{\alpha i}$, with group structure $U(4)\otimes U(n)$. The associated algebraic problem can be solved either on a computer, or, in some simpler cases, analytically. Work in this direction is in progress.

In conclusion, I have pointed out that, if moleculariike states are formed in heavy-ion collisions, the structure of the corresponding spectrum should be rather different from that observed in the low-lying spectra of nuclei. I have also proposed a new approach to the study of molecular spectra, based on the use of algebraic techniques. I have presented a simple application of these techniques and suggested a possible way to extend them to more complex situations.

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