Algebraic Approach to Dissociation from Bound States

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An algebraic treatment of continuous spectra based on noncompact groups is extended to allow discussion of dissociation from bound states. Transition matrix elements between bound and continuum states can be evaluated algebraically by the construction of transition operators that transform according to the infinite-dimensional unitary representations of the noncompact dynamical group. The method is employed to calculate dissociation rates in the Morse potential, for which the relevant group is SO(2,1).

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Recently, the algebraic approach to bound states, useful in nuclear[1] and molecular[2] physics, has been extended to the continuum.[3,4] In bound-state problems, a major advantage of the algebraic approach is the easy evaluation of transition matrix elements such as those related to electromagnetic decay. The inclusion of the continuum opens a new and interesting problem, namely the algebraic evaluation of transition matrix elements between bound and scattering states. These quantities describe the probability that a system will dissociate from some bound level into fragments with a given relative kinetic energy.

By using what we call the "potential algebra," which is noncompact, we were able to unify the treatment of bound and scattering spectra; the discrete representations of a system's noncompact algebra describe its bound states while the continuous principal-series representations correspond to its continuum states.[4] The purpose of this Letter is to demonstrate that this algebra can be used to calculate dissociation rates; to the best of our knowledge, these have been evaluated analytically only for the Coulomb potential,[5] through very different techniques from the ones to be presented here. Our basic idea is to construct transition operators that transform like irreducible tensors under the potential group, and then use a Wigner-Eckart theorem carefully adapted to noncompact algebras. An important conclusion will be that in order to obtain finite nonvanishing matrix elements between bound and continuum states, particular classes of tensor operators must be employed. The finite-dimensional nonunitary representations, though they provide simple selection rules for bound-to-bound transitions,[6] are unsuitable for dissociation.

As in some of our previous investigations, we shall illustrate our ideas with a discussion of a simple one-dimensional system possessing SO(2,1) symmetry, in this case the Morse potential.[7] The Hamiltonian is obtained from the SO(2,1) realization[8]

$$J_{\pm} = e^{\pm i\phi}[\mp \partial/\partial\rho - i\,\partial/\partial\phi - e^{-\rho} \pm \tfrac{1}{2}],$$
$$J_z = -i\,\partial/\partial\phi. \tag{1}$$

The basis states corresponding to the dynamical symmetry $SO(2,1)\supset SO(2)$ are characterized by

$$C|j,m\rangle = j(j+1)|j,m\rangle, \quad J_z|j,m\rangle = m|j,m\rangle, \tag{2}$$

where $C = J_z^2 - (J_+J_- + J_-J_+)/2$ is the Casimir invariant of the algebra. In the realization (1) they describe eigenstates of a Schrödinger equation

$$[-\partial^2/\partial\rho^2 + (e^{-2\rho} - 2me^{-\rho})]u_m^j(\rho) = -(j+\tfrac{1}{2})^2 u_m^j(\rho), \tag{3}$$

where $|j,m\rangle = u_m^j(\rho)e^{im\phi}$. A simple translation $\rho \rightarrow \rho - \ln(m)$ takes Eq. (3) into that for a Morse potential, $V = m^2(e^{-2\rho} - 2e^{-\rho})$.

The following SO(2,1) unitary irreducible representations appear in (2): (a) the discrete representations D_j^+ with $j = -\frac{1}{2}, -1, -\frac{3}{2}, \ldots$ and $m = -j, -j+1, -j+2, \ldots$, describing bound states with energy $E = -(j+\frac{1}{2})^2$, and (b) the continuous principal-series representations C_j^{δ} with $j = -\frac{1}{2} + ik$, $k > 0$, and $m = 0, \pm 1, \pm 2, \ldots$ for $\delta = 0$ and $m = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$ for $\delta = \frac{1}{2}$, corresponding to continuum states with energy $E = k^2$. Within a given representation the energy is constant but the strength of the potential changes—hence the name "potential algebra."

To calculate bound-state–to–bound-state and bound-state–to–continuum transitions we employ SO(2,1) tensor operators (the generators themselves will not connect different representations). The first class of operators that suggests itself transforms according to the simple finite-dimensional nonunitary SO(2,1) representations D_j. These representations, which correspond to the well-known unitary representations of SO(3), have $j = \frac{1}{2}, 1, \frac{3}{2}, \ldots$ and $m = -j, -j+1, \ldots, j$. Operators T_m^j transforming according to them have been successfully used to calculate bound-bound transition matrix elements in the Coulomb and harmonic-oscillator problems.[9,10] Consider transitions induced by such operators between states corresponding to different potentials (such transitions are important, for example, in the description

of molecular transitions during which the electronic configurations change). Suppose that the initial state $|j_1,m_1\rangle$ is bound and therefore belongs to the representation $D_{j_1}^+$; it has energy $-(j_1+\frac{1}{2})^2$ and is associated with a potential of strength m_1. The final state $|j_3,m_3\rangle$ has energy $-(j_3+\frac{1}{2})^2$, belongs to a potential of strength m_3, and can be either a bound or continuum state. We want to evaluate the matrix elements of T^{j_2} between these two objects. The states obtained by operating on the $|j_1,m_1\rangle$ with the tensor operator T^{j_2} above form a basis for the Kronecker product representation $D_{j_1}^+ \times D_{j_2}$. Its decomposition into irreducible representations, given by Wybourne,[11] contains D_j^+, and D_j in addition when the initial state is one of the higher-lying levels. The former clearly have no overlap with the continuum states. The latter, while they are nonunitary and therefore not automatically orthogonal to the C_j representations, can be shown to yield divergent amplitudes when projected onto the continuum states. We therefore conclude that for the Morse potential, tensors belonging to the D_j representations can never produce finite nonvanishing matrix elements for dissociation processes.

This result leads us to consider tensor operators transforming under one of the infinite-dimensional unitary representations[11] of SO(2,1), either $D_j^{\pm}$ or C_j^{δ}. For these representations, the shift operators act as follows:

$$[J_{\pm},T_m^j]=[(j\pm m)(m\pm j\pm 1)]^{1/2}T_{m\pm 1}^j,$$
$$[J_z,T_m^j]=mT_m^j. \tag{4}$$

In the Morse realization the momentum-independent tensors turn out to be given by

$$T_m^j=[\Gamma(-j-m)/\Gamma(j-m+1)]^{1/2}e^{j\rho}e^{im\phi}. \tag{5}$$

The matrix element we wish to evaluate then takes the form

$$\langle j_3,m_3|T_{m_2}^{j_2}|j_1,m_1\rangle \propto \int_{-\infty}^{\infty}d\rho\, u_{m_3}^{j_3*}(\rho)e^{j_2\rho}u_{m_1}^{j_1}(\rho), \tag{6}$$

where $m_2=m_3-m_1$.

Since j_2 is <0 (for the discrete series) or is complex ($j_2=-\frac{1}{2}+ik$ for continuous series), we should now obtain finite bound-continuum matrix elements. However, the Kronecker product for the coupling of two D^+ representations[12] yields only D^+'s; thus while a tensor belonging to one of these will connect bound states, it is useless for dissociative processes. The coupling of D^+ and D^- yields both the D^+ (with some restrictions of the range of j) and the C series, so that we do expect to be able to connect bound and continuum states using D^- tensor operators.[13] This case will be discussed in more detail in a longer paper. For the rest of this work we shall discuss transition operators transforming according to the representations C_j^0, which always include an $m=0$ component.

The Kronecker product appropriate for these transitions yields under decomposition

$$D_{j_1}^+ \otimes C_{j_2}^0=\sum_{j_3=-1}^{-\infty}D_{j_3}^+ +\int_{-1/2-i\infty}^{-1/2+i\infty}dj_3\,C_{j_3}^0 \tag{7}$$

(a similar decomposition exists for $C_j^{1/2}$). Thus a tensor that transforms according to one of the C representations can connect a bound state j_1 to *every* bound or continuum state j_3. The $m=0$ component corresponds to the important special case in which the potential strength does not change during the transition. We recall that for the continuous representations $j_2=-\frac{1}{2}+i\kappa$, so that in a coordinate representation the operator is proportional to $e^{-\rho/2}e^{i\kappa\rho}$.

We turn now to the algebraic evaluation of the transition matrix elements. The procedure is based on the Wigner-Eckart theorem, which may be extended to noncompact groups like SO(2,1) provided that no degeneracy occurs in the Kronecker product and all the representations involved are orthogonal to one another. Like its SU(2) angular-momentum-coupling counterpart, the theorem states that

$$\langle j_3,m_3|T_{m_2}^{j_2}|j_1,m_1\rangle = \langle j_1m_1,j_2m_2|j_3m_3\rangle\langle j_3||T^{j_2}||j_1\rangle. \tag{8}$$

This equation expresses the fact that the m (potential) dependence of the matrix element is completely determined by the SO(2,1) Clebsch-Gordan coefficient $\langle j_1m_1,j_2m_2|j_3m_3\rangle$. Thus, once we know that matrix element for one case we know it for all cases.

SO(2,1) Clebsch-Gordan coefficients for the coupling of the various different kinds of representations have been extensively investigated.[12,14] They can be obtained from recursion relations[15] and turn out always to be proportional to a generalized hypergeometric function ${}_3F_2$ of unit argument (the study of these objects was systematized by Whipple long ago[16]). The coefficient in which we are interested at the moment is given in equation (2.37) of Ref. 12. Using symmetry relations for the ${}_3F_2$'s, we write it in the form

$$\langle j_1m_1,j_2m_2|j_3m_3\rangle=\frac{\alpha(j)}{\Gamma(m_2-j_1-j_3)}\left[\frac{\Gamma(m_1-j_1)\Gamma(m_3-j_3)}{\Gamma(m_1+j_1+1)\Gamma(m_3+j_3+1)\Gamma(-m_2+j_2+1)\Gamma(-m_2-j_2)}\right]^{1/2} \times {}_3F_2(-m_1-j_1,-j_1+j_2-j_3,-j_1-j_2-j_3-1;m_2-j_1-j_3,-2j_1;1), \tag{9}$$

where $\alpha(j)$ is a complicated function that does not depend on the m's and therefore will divide out in the application of Eq. (8). This form of the coefficient has the advantage that neither the Γ functions nor the ${}_3F_2$ function have poles at the points at which we evaluate them. Further, since $-m_1-j_1$ is always negative, the expansion of the ${}_3F_2$ function involves only a finite number of terms, and is readily evaluated numerically.

To complete the calculation we need an expression for the reduced matrix element, or equivalently for the complete matrix element given one particular choice of the m quantum numbers. This quantity is not determined by the potential algebra but can be evaluated analytically for the Morse oscillator having values of m for which the wave functions simplify. The ground state of the Hamiltonain has the simple form[17] (with $x=2e^{-\rho}$)

$$|j,-j\rangle e^{-x/2}x^{-(j+1/2)}e^{-j\phi}/[2\pi\Gamma(-2j)]^{1/2}.$$

Furthermore, when $m=0$, the Schrödinger problem corresponds to the especially simple potential $V=e^{-2\rho}$. The solutions then take the form $\psi_0^j=K_{j+1/2}(x/2)/[\pi\Gamma(-j-\frac{1}{2})]^{1/2}$, where K is a Bessel function of fractional order $j+\frac{1}{2}=ik$; ψ is a normalized scattering solution with energy k^2. Using these to calculate the overlap integral, we find for the reduced matrix element of the bound (j_1) to continuum ($j_3=-\frac{1}{2}+ik$) transition

$$\langle j_3||T^{j_2}||j_1\rangle=\frac{\langle j_3,0|T^{j_2}_{j_1}|j_1,-j_1\rangle}{\langle j_1-j_1,j_2j_1|j_30\rangle}$$

$$=\frac{2^{j_2+1/2}}{\alpha(j)}\Gamma(-j_1-j_2+j_3)\Gamma(-j_1-j_2-j_3-1)\left[\frac{\Gamma(j_3+1)\Gamma(-j_3)}{\Gamma(-2j_1)\Gamma(-2j_1-1)}\right]^{1/2}. \tag{10}$$

We may now combine (8)–(10) to obtain for the bound-state–continuum transition matrix element the result

$$\langle j_3,m_3|T^{j_2}_{m_2}|j_1,m_1\rangle=\frac{2^{j_2+1/2}}{\Gamma(j_3+\frac{1}{2})}\frac{\Gamma(-j_1-j_2+j_3)\Gamma(-j_1-j_2-j_3-1)}{\Gamma(m_2-j_1-j_3)}$$

$$\times\left[\frac{\Gamma(m_1-j_1)\Gamma(m_3-j_3)\Gamma(j_3+1)\Gamma(-j_3)}{\Gamma(m_1+j_1+1)\Gamma(m_3+j_3+1)\Gamma(-m_2+j_2+1)\Gamma(-m_2-j_2)\Gamma(-2j_1)\Gamma(-2j_1-1)}\right]^{1/2}$$

$$\times{}_3F_2(-m_1-j_1,-j_1+j_2-j_3,-j_1-j_2-j_3-1;m_2-j_1-j_3,-2j_1;1). \tag{11}$$

Bound-bound transitions may be evaluated in a completely analogous fashion.

For transitions from the ground state ($m_1=-j_1$) the hypergeometric function in (11) is equal to 1. Since we have normalized the continuum states in the usual way [to $\delta(k-k')$], it is clear that the square of (11) is just the transition probability density in momentum space. If we are interested in the distribution versus energy, we have to multiply the square of (11) by the energy-level density, which in one dimension is $1/\sqrt{E}$. In Fig. 1 we have plotted the distribution of transition probabilities over the bound and continuum states for a particular choice of the transition operator. The location of the peak in the continuum is sensitive to the imaginary part κ of the tensor label j_2. The strength at $E=0$ always vanishes because of the properties of the zero-energy wave function.

We note in passing that independent of the value of j_2, the transition strength to all the bound and continuum states sums to $-(j_1+\frac{1}{2})$, the expectation value in the ground state of the operator T with $j_2=-1$. A similar energy-weighted sum rule can also be derived by considering the commutator of the Casimir operator (the Hamiltonian up to a constant) with T.

There appears to be a range of applications for the techniques described in this Letter. Transition operators similar to the ones considered here appear in atomic ionization processes resulting from collisions with fast electrons.[18] Operators of the form $e^{j\rho}$ (j real) have also been used in the analysis of dipole (bound-to-bound) transitions in molecules.[17] Furthermore, the tensor operators discussed here can be seen to form a complete set so that arbitrary transition operators may be expanded in the T's. Finally, our ideas apply naturally in algebraic models incorporating angular momentum of the kind discussed, e.g., by Alhassid, Iachello, and Wu.[19] These may be useful in modeling complex problems in molecular and atomic physics, where prospects for an algebraic treatment of

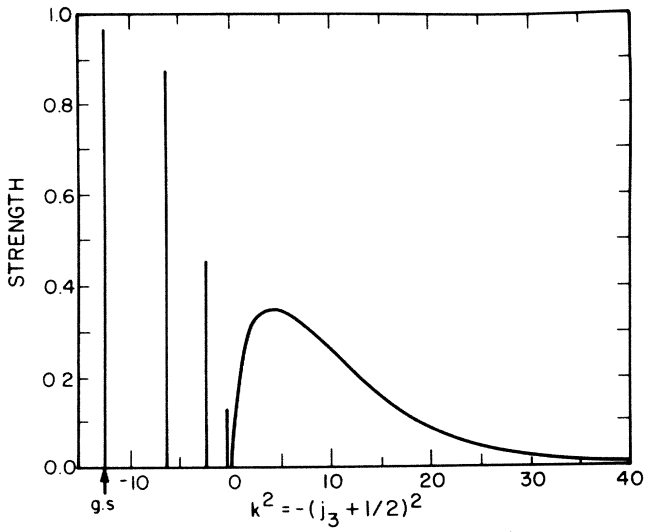

FIG. 1. The transition strength ($|\langle j_3,m_3|T^{J_2}_{m_2}|j_1,m_1\rangle|^2$) from the ground state ($j_1 = -m_1$) of a Morse potential with four bound states ($m_1 = 4$) to excited states, including the continuum, of the same potential ($m_3 = m_1$) plotted vs excited state energy $E = -(j_3 + \frac{1}{2})^2$. The transition operator is given in Eq. (5) with $j_2 = -\frac{1}{2} + 3i$. The first line is the ground-ground diagonal strength. The probability density $P(E)$ for transitions to the continuum is obtained by multiplying the strength by the density of states $1/\sqrt{E}$.

dissociation seem most promising.

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