

Resonance Widths and Positions by an Algebraic Approach

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The use of nonunitary discrete, irreducible representations of Lie algebras is proposed as a method for the determination of widths and energies of resonances. The method is illustrated by explicit application to three kinds of resonances: in transmission over a well, in transmission over a barrier, and in barrier penetration for a family of one-dimensional potentials. The same procedure is also useful in an algebraic approach to scattering by a complex (optical) potential, and for parametrization of the resonant contribution to the scattering matrix.

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Algebraic techniques have proven useful in the description of bound states in nuclear¹ and molecular² physics. Recently, we have considered an algebraic description of the continuous spectrum^{3,4} and the computation of the scattering matrix.^{5,6} An important aspect of many scattering problems is the appearance of resonances. These resonances can be identified as poles of the S matrix, below the real positive energy axis (in the second Riemann sheet, corresponding to the lower half of the momentum plane; $E = k^2$, $\text{Im}k < 0$). These resonances are known to correspond to quasibound states of the system whose energy is in the continuum. By the enforcing of a purely discrete spectrum such resonances can be approximated as bound states (whose width is then necessarily zero) and such an approximation is possible also in the algebraic approach.^{2,7} The question is whether the *quasi-*

bound states can be described exactly by algebraic techniques.

The purpose of this Letter is to argue that an algebraic approach to resonances as quasibound states is feasible. We shall, for simplicity, consider one-dimensional problems. Explicit results for the widths and positions of resonances will be provided for a class of potentials for which an exact correspondence between the coordinate representation and the algebraic form exists. The essential new tool is the use of discrete but nonunitary representations.

In this Letter we restrict our attention to one-dimensional systems. In configuration space such systems describe two channels (L, R) which correspond to the (asymptotic) left- and right-hand-side regions. At any given energy $E = k^2$ one can construct a unique scattering state which describes a wave incident from the left:

$$\psi(\rho) \rightarrow \begin{cases} A(E)\exp(ik\rho) + B(E)\exp(-ik\rho), & \rho \rightarrow -\infty, \\ \exp(ik\rho), & \rho \rightarrow \infty. \end{cases} \quad (1)$$

The condition for a resonance is purely outgoing waves in both channels,^{8,9} namely, $A(E) = 0$. Such boundary conditions correspond to a decaying state and violate the conservation of flux. The energies which are the solutions of $A(E) = 0$ are a discrete set of complex eigenvalues, $E = E_0 - i\Gamma/2$. The real part, E_0 , is interpreted as the resonance energy and Γ is the resonance width. We shall propose a purely algebraic procedure which corresponds to the above coordinate-space approach.

We illustrate the approach by examples based on the following consideration. For several classes of one-dimensional potentials, the group $SU(1,1)$ plays the role of a potential group.^{3,6} That means that the basis for an irreducible representation¹⁰ is provided by a set of eigenstates, all at a common, fixed, energy, which correspond to different values for the strength param-

eter of the potential. The bound states are obtained as the basis of a discrete-series representation of $SU(1,1)$, while the scattering states belong to a continuous-series representation.^{4,11} Both types of representations are unitary as is required by the Hermiticity of the Hamiltonian and the boundary conditions. For a quasibound state the boundary conditions correspond to a nonunitary representation. The energy eigenvalues in such a nonunitary representation can be complex. For a Hamiltonian with a dynamical symmetry these complex energies can be determined analytically. Both the widths and positions of the resonances can thus be calculated in the proposed algebraic approach. Since the spectrum of quasibound states is discrete, the relevant nonunitary representations will be discrete. Explicit examples for the $SU(1,1)$ group

are provided below.

We consider the SU(1,1) dynamical algebra with generators J_{\pm}, J_z :

$$[J_z, J_{\pm}] = \pm J_{\pm}, \quad [J_+, J_-] = -2J_z. \quad (2)$$

When the Hamiltonian has a dynamical symmetry it is a function (we shall use a linear function) of the Casimir invariant $C = J_z^2 - (J_+ J_- + J_- J_+)/2$ of the group. Hence, for systems with dynamical symmetry we shall simultaneously diagonalize the Casimir invari-

ant and the generator J_z ,

$$C|j, m\rangle = j(j+1)|j, m\rangle, \quad J_z|j, m\rangle = m|j, m\rangle. \quad (3)$$

In the applications below where SU(1,1) is a potential group, $|j, m\rangle$ is an energy eigenstate with an energy determined by j for a potential characterized by the parameter m .

To examine quasibound states of different types we consider a class of potentials which was recently studied (in configuration space) by Ginocchio.¹² This class of potentials corresponds to the following¹³ realization of SU(1,1):

$$J_{\pm} = \exp(\pm i\phi) \frac{\pm(\partial/\partial r) \pm (\lambda^2 - 1)y(1 - y^2)/2 + \lambda y[-i(\partial/\partial\phi) \pm \frac{1}{2}]}{\lambda[\lambda^2 + (\lambda^2 - 1)y^2]^{1/2}}, \quad J_z = -i(\partial/\partial\phi), \quad (4)$$

where y is a function of r defined by

$$r = [\operatorname{invtanh}y - (1 - \lambda^2)^{1/2} \operatorname{invtanh}y(1 - \lambda^2)^{1/2}y]/\lambda^2 \quad (5)$$

and λ is a constant. The proof that the generators given by (4) do satisfy the defining commutation relations (2) is tedious but feasible.

The solution of the algebraic eigenvalue equations (3),

$$\langle r, \phi | j, m \rangle = \psi_{jm}(r) \exp(im\phi),$$

leads to the Schrödinger equation

$$[-(d^2/dr^2) + V_m(r)]\psi_{jm}(r) = -\lambda^4(j + \frac{1}{2})^2\psi_{jm}(r), \quad (6)$$

with an m -dependent potential

$$V_m(r) = -\lambda^2\nu(\nu + 1)(1 - y^2) - (\lambda^2 - 1)(1 - y^2)[5(1 - \lambda^2)y^4 + (\lambda^2 - 7)y^2 + 2]/4. \quad (7)$$

In (7), the parameter ν depends on m (and λ and j) via

$$(\nu + \frac{1}{2})^2 = m^2 + (\lambda^2 - 1)(j + \frac{1}{2})^2. \quad (8)$$

The potential $V_m(r)$ as given by (7) depends on two parameters ν and λ which determine the number of bound states and the shape of the bottom of the potential, respectively.¹² In the algebraic description, λ has a fixed value. A given representation of SU(1,1) corresponds to a fixed j . A basis $|j, m\rangle$ of states for a given representation corresponds therefore to a set of eigenstates, all having the same energy [i.e., $-\lambda^4(j + \frac{1}{2})^2$], which belong to potentials $V_m(r)$, as given by (7) with varying strength parameters $\nu = \nu_m$. The values of ν for the set of allowed m values are given by (8).

The discrete representations¹⁰ D_j^+ of SU(1,1) are characterized by

$$m = -j, -j + 1, -j + 2, \dots \quad (9)$$

When j is real, these representations are unitary (single or multivalued) and describe bound states at energies

$$E = -\lambda^4(j + \frac{1}{2})^2. \quad (10)$$

For a complex j , $j = \alpha + i\beta$, the representation D_j^+ is

nonunitary although still discrete.¹⁰ The eigenenergies are still given by (10) except that they are now complex, $E = E_0 - i\Gamma/2$, where

$$E_0 = \lambda^4[\beta^2 - (\alpha + \frac{1}{2})^2], \quad \Gamma = 4\lambda^4(\alpha + \frac{1}{2})\beta. \quad (11)$$

For $|\beta| > |\alpha + \frac{1}{2}|$ and $\beta(\alpha + \frac{1}{2}) > 0$, (11) defines a resonance of positive energy E_0 and width Γ . For $E_0 < 0$, $\Gamma = 0$ and the states are virtual bound states. Note that E_0 and Γ depend only on the real and imaginary parts of j but not on m .

The nonunitary representation D_j^+ with a complex j has as its basis $|j, m\rangle$ a set of resonances of constant position E_0 and constant width Γ , belonging to a series of potentials (7) with m given by (8). The ladder operators J_{\pm} step m by units of ± 1 , as usual. That the set of resonances above spans one irreducible representation of SU(1,1) is a consequence of an important implication of the realization (4) of the ladder operators: They preserve the boundary condition $A(E) = 0$ which defines a resonance in terms of the asymptotic form (1) of the scattering wave function. This can be seen directly by taking the asymptotic form of the ladder operators. The asymptotic expression preserves the outgoing character of the wave in the left-hand ($y \rightarrow -1$) and right-hand ($y \rightarrow 1$) sides.

The algebraic determination of the sequence of resonances of a *given* potential (λ and ν fixed) is now readily carried out, as follows. For a fixed ν and for a given set, (10), of allowed values of m , $m = -j + n$ ($n = 0, 1, 2, \dots$), (9) provides a quadratic equation for j whose solution is

$$\lambda^2(j + \frac{1}{2}) = + i[(\lambda^2 - 1)(n + \frac{1}{2})^2 - \lambda^2(\nu + \frac{1}{2})^2]^{1/2}.$$

Comparing with (10) we have for a given potential

$$E_{0n} = (\lambda^2 - 2)(n + \frac{1}{2})^2 - \lambda^2(\nu + \frac{1}{2})^2, \quad \Gamma_n = 2(2n + 1)[(\lambda^2 - 1)(n + \frac{1}{2})^2 - \lambda^2(\nu + \frac{1}{2})^2]^{1/2}. \quad (12)$$

When $\lambda^2 > 2$ and n is large enough so that $E_{0n} > 0$, (12) specifies the positions and widths of the resonances. Potentials of the form (7) with $\lambda^2 > 2$ resemble the Pöschl-Teller¹⁴ form ($\lambda = 1$) but are flatter at the bottom. As λ increases, their form resembles a square well which is well known to have resonances in its transmission. For the potential (7), the asymptotic form of the scattering wave function in configuration space can be analytically determined.¹² We have verified [see also the discussion of (14) below] that the energies and widths (12) are the very same as those determined from the boundary condition $A(E) = 0$ imposed on the scattering solution (1). Here of course, the resonance positions and widths have been determined in a purely algebraic fashion.

For the resonances (12) to be sharp ($\Gamma_n \ll E_{0n}$) and nonoverlapping ($\Gamma_n < E_{0n+1} - E_{0n}$) we need to have roughly $\lambda\nu^{1/2} \gg 1$. Figure 1 shows the well for $\nu = 12$, $\lambda = 12$, and the transmission coefficient versus energy. [Energy is measured in units of the well depth $V(0)$.] The resonances that we have so far discussed have therefore a clear scattering interpretation in terms of the transmission (at positive energies) across

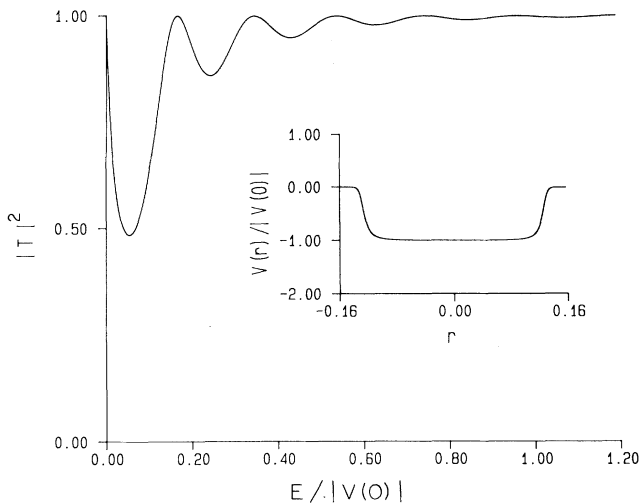


FIG. 1. The transmission coefficient vs energy [in units of the potential depth $V(0)$] for the potential well $V(r)$ shown vs r in the inset. The potential $V(r)$ is given by (7) with $\lambda = 12$ and $\nu = 12$, and $|T|^2$ is computed from (14). The resonances in transmission across the well are quite evident.

the well.

Another type of resonance is for transmission across a barrier. A suitable class of potentials is again given by (7) except that now we take ν to be complex and specifically $\nu = -\frac{1}{2} + i\eta$, so that $\nu(\nu + 1) = -\eta^2 - \frac{1}{4}$. The potential (7) remains real but now describes a barrier. The positions and widths are here, too, given by (12).

Finally we come to the more familiar type of resonance in one-dimensional systems—a particle trapped within a hollow.¹⁵ A suitable class of potentials is again given by (7) provided that $\lambda \gg \nu$ (or $\lambda \gg \eta$). The resonances are given by (12). Figure 2 shows the potential and the resonances in the transmission.

Work is in progress along several directions. First, there is the extension to more degrees of freedom. Once we allow two or more spatial coordinates, a new type of resonance is possible. These, sometimes called “closed channel” resonances,¹⁶ are due to a coupling which when turned off leaves a bound state embedded

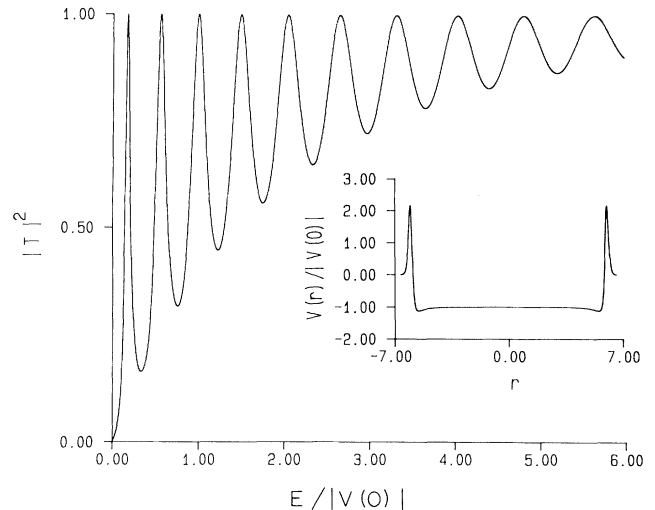


FIG. 2. Same as Fig. 1 but for $\lambda = 26$ and $\nu = 5.5$. There are now five resonances at positive energies which, for much thicker barriers, would be practically bound states. Their formation and decay is via tunneling through the barriers. Note that the width of the resonance increases as its decay (or formation) requires penetration through a thinner barrier.

in a continuum. Such resonances have already been approximated in an algebraic approach as bound states.⁷ The algebraically computed energies of such bound states compare quite well with the positions of the resonances determined via a scattering computation¹⁷ (in configuration space). It remains, however, to determine the widths of such resonances by an algebraic approach.

This Letter has emphasized the use of nonunitary but discrete representations for the determination of resonances. The unitary but continuous representations are spanned by the scattering states of potentials which are real valued.^{3,4,11} It proves possible to use nonunitary and continuous representations for the scattering by complex-valued (e.g., optical) potentials and further work is forthcoming.

In terms of understanding the fundamentals it should prove worthwhile to establish the connection between the present algebraic approach and the recently much studied¹⁸ configuration-space procedure based on complex scaling [$r \rightarrow r \exp(i\theta)$] of the coordinates and sometimes known as "dilation analyticity."

Finally, an interesting potential application is towards a parametrization of the scattering matrix in terms of the resonances, and the bound states.⁸ On the practical level, for an isolated resonance which is near the real axis, the resolution of the scattering matrix element into a slowly varying background term and a Breit-Wigner-type resonant term is useful,

$$S_{ij} = S_{ij}^0 - i\gamma_i\gamma_j(E - E_0 - i\Gamma/2). \quad (13)$$

Here $|\gamma_i|^2$ is the partial width in the i th channel and S^0 is the background contribution. The transition probability will, in general, manifest interference between the background and resonant terms in the amplitude and so an algebraic parametrization for the background term is necessary. The present examples (cf. Figs. 1 and 2) are for reflection symmetric potentials where one can show (e.g., using WKB wave functions) that the interference term vanishes at the resonance energies. Hence at the vicinity of the resonance energy the transmission coefficient should have a pure Breit-Wigner form and equal exactly unity at E_0 . This behavior is nicely reproduced in the exact results shown in Figs. 1 and 2. The expression for $|T|^2$ can be analytically determined¹² and can also be derived by algebraic means¹³ through the continuous unitary representation of $SU(1,1)$. The result is,¹² in the present notation,

$$|T|^2 = \left| \frac{\Gamma(m-j)\Gamma(-m-j)}{\Gamma(-\frac{1}{2}-j)\Gamma(\frac{1}{2}-j)} \right|^2, \quad (14)$$

where $\Gamma(z)$ is the gamma function. j is related to the

energy $E = k^2$ by $j = -\frac{1}{2} + ik/\lambda$ [cf. (11)]. Inspection of (14) suggests that even the longer-range goal,⁸ namely, a parametrization of the energy dependence of the scattering matrix entirely through its singularities, may be possible by algebraic means.

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