Potential Scattering, Transfer Matrix, and Group Theory

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Both bound and scattering states of the Pöschl-Teller potential are shown to be connected with unitary representations of certain groups. A family of periodic potentials, and their associated transfer matrices and band structure, can also be obtained from group theory and reduce to the above potential when the real period approaches infinity. These results suggest that the algebraic approach used for treating bound-state problems can be extended to scattering and band-structure problems.

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Group theory has wide applications in physics. While symmetry groups can account for degeneracies of levels and selection rules, dynamical groups are useful in generating the spectra and reducing the calculation of certain transition matrix elements to algebraic manipulations. In the last few years, dynamical algebras have been used extensively to describe the spectra of a variety of physical systems, such as collective states in nuclei[1] and rotation-vibration spectra in molecules.[2] However, these applications were restricted to bound states. In this paper, we provide the first steps towards their extension to the other two types of spectra observed in physical systems, continuous and band structures (in periodic potentials). The inclusion of the continuum is important when we wish to study scattering processes as well as dissociation.

In order to illustrate the connection between group theory and (bound and scattering) states in a potential, we consider the Pöschl-Teller[3] potential, $-V_0/\cosh^2\rho$, that appears in a variety of physical situations. It emerges as the mean field of a many-body system with a δ-function two-body force,[4] as the nonrelativistic limit of the sine-Gordon equation,[5] and in connnection with completely integrable many-body systems in one dimension.[6] We shall show that the bound states of this potential, finite in number, form a basis for a representation of SU(2). The scattering states are obtained by an analytic continuation to the noncompact group[7] SU(1, 1). The latter has unitary representations associated with a spectrum that can be continuous. This appears to be a general result: Whenever the bound states are describable by representations of a compact group, the scattering states are obtained by an analytic continuation to the continuous representations of a corresponding noncompact group.

The Pöschl-Teller potential corresponds to a dynamical symmetry of the associated algebra. If we consider the most general algebraic Hamiltonian quadratic in the generators (thus relaxing the condition of a dynamical symmetry), we obtain a family of periodic potentials. These potentials are of interest in solid-state physics, as they describe models for crystals that are more realistic than the well-known Kronig-Penney[8] and Scarf[9] potentials. It is found that the group provides us with a band structure and with the standing Bloch solutions at the center and the edges of the Brillouin zone. The (nonperiodic) Pöschl-Teller potential can be obtained by continuously deforming the periodic potentials as their real period approaches infinity. In this process, the bandwidth shrinks to zero so as to produce sharp bound states.

To begin with, consider the group SU(2) generated by the three operators J_x, J_y, J_z, and the Hamiltonian $H=-J_z^2$. If we diagonalize H in the subspace of a given irreducible representation, where the Casimir invariant $C=\vec{J}^2$ is a constant, we obtain the set of equations

$$H\Psi_j{}^m = E_m\Psi_j{}^m, \quad C\Psi_j{}^m = j(j+1)\Psi_j{}^m. \tag{1}$$

These equations can be realized in spherical coordinates (r, θ, φ), where the operators J_x, J_y, J_z have their usual form obtained from $\vec{J} = \vec{r}\times(-i\nabla)$. The solutions then separate and are given by $\Psi_j{}^m(\theta, \varphi) \propto e^{im\varphi}P_j{}^m(\cos\theta)$, with energies $E_m = -m^2$. The associated Legendre functions $P_j{}^m(\cos\theta)$ satisfy a well-known differential equation which, upon the substitution $\cos\theta = \tanh\rho$ $(-\infty < \rho < +\infty)$, transforms to the Schrödinger equation for the bound states of the Pöschl-Teller potential,

$$\left(-\frac{d^2}{d\rho^2} - \frac{j(j+1)}{\cosh^2\rho}\right)P_j{}^m(\rho) = -m^2P_j{}^m(\rho). \tag{2}$$

The strength of the potential V_0 is given by $j(j+1)$.

The analytic continuation to the equation satisfied by the scattering states could be formally obtained from Eq. (2), by the substitution $m \to ik$. However, the group wave functions will then have the wrong φ dependence. In order to obtain the correct dependence, we must, at the same time, analytically continue the group SU(2) to its noncompact version, SU(1, 1). This is done simply by introducing the operators

$$\begin{aligned} I_x &= i\left(y\frac{\partial}{\partial z} + z\frac{\partial}{\partial x}\right),\\ I_y &= -i\left(z\frac{\partial}{\partial z} - x\frac{\partial}{\partial z}\right),\\ I_z &= -i\left(x\frac{\partial}{\partial y} + y\frac{\partial}{\partial x}\right). \end{aligned} \tag{3}$$

These operators satisfy the SU(1, 1) commutation relations, $[I_x, I_y] = iI_z$, $[I_y, I_z] = iI_x$, $[I_z, I_x] = -iI_y$. Furthermore, instead of spherical coordinates, we introduce hyperbolic coordinates,

$$\begin{aligned} &x = r\sin\theta\cosh\varphi, \quad y = r\sin\theta\sinh\varphi,\\ &z = r\cos\theta, \end{aligned} \tag{4}$$

where $0 \leqslant \varphi < \infty$. The sphere of radius r is thus continued to the hyperboloid $x^2 - y^2 + z^2 = r^2$. We now solve the set of equations

$$H\Psi_j{}^k = E_k\Psi_j{}^k, \quad C\Psi_j{}^k = j(j+1)\Psi_j{}^k, \tag{5}$$

where C is the Casimir invariant of SU(1, 1), $C = -I_x{}^2 + I_y{}^2 - I_z{}^2$, and $H = I_z{}^2$, $E_k = k^2$. This Hamiltonian has a continuous spectrum characterized by the continuous eigenvalues, k, of the noncompact generator,[7] I_z. Using (4) we still find $I_z = -i\,\partial/\partial\varphi$, so that the realization of Eq. (5) in hyperbolic coordinates separates, $\Psi_j{}^k(\theta, \varphi) \propto e^{ik\varphi}R_j{}^k(\cos\theta)$, and the functions $R_j{}^k(\cos\theta)$ satisfy an equation, which, after the transformation $\cos\theta = \tanh\rho$ yields the Schrödinger equation for the scattering states of the Pöschl-Teller potential with momentum k,

$$\left(\frac{d^2}{d\rho^2} - \frac{j(j+1)}{\cosh^2\rho}\right)R_j{}^k(\rho) = k^2R_j{}^k(\rho). \tag{6}$$

The functions $R_j{}^k(\rho)$ are obtained from the Legendre functions by analytic continuation, $R_j{}^k(\rho) \propto P_j{}^{ik}(\tanh\rho)$.

It is interesting to note that the scattering, S, and transfer, M, matrices for this problem can be written in closed form. In order to do this, it is sufficient to consider the asymptotic form of the solutions $R_j{}^k(\rho)$ as $\rho \to \pm\infty$. For any localized potential, one can write the most general scattering solution at $\rho \to \pm\infty$ as

$$\begin{aligned} &R(\rho) \to A_0e^{ik\rho} + B_0e^{-ik\rho}, \quad \rho \to -\infty,\\ &R(\rho) \to A_1e^{ik\rho} + B_1e^{-ik\rho}, \quad \rho \to +\infty. \end{aligned} \tag{7}$$

The scattering matrix S transforms the two incoming waves with amplitudes A_0, B_1 into the two outgoing waves with amplitudes B_0, A_1. For a real potential, conservation of flux $|A_0|^2 + |B_1|^2 = |A_1|^2 + |B_0|^2$ implies unitarity of S. Thus S is a U(2) matrix. Similarly, the transfer matrix M transforms the amplitudes at $\rho \to -\infty$, A_1, B_1, into the amplitudes at $\rho \to +\infty$, A_0, B_0. Since $|A_0|^2 - |B_0|^2 = |A_1|^2 - |B_1|^2$, M is quasiunitary and since, in addition, $\det M = 1$, M is an SU(1, 1) matrix. The matrix elements of M can be obtained from those of S and vice versa. One finds that, for the Pöschl-Teller potential,

$$\begin{aligned} M &= \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix},\\ \alpha &= \frac{\Gamma(ik)\Gamma(1+ik)}{\Gamma(1+ik+j)\Gamma(ik-j)},\\ \beta &= \frac{\Gamma(ik)\Gamma(1-ik)}{\Gamma(-j)\Gamma(j+1)}. \end{aligned} \tag{8}$$

For a scattering potential, M contains equivalent information to S. However, it is the transfer matrix M which is naturally generalized to the case of periodic potentials.

Our discussion so far has been confined to cases that can be described by a dynamical symmetry,[1,2] i.e., cases in which the Hamiltonian is written in terms of invariant operators of a complete chain of groups, SU(2) ⊃ SO(2) and SU(1, 1) ⊃ SO(1, 1), respectively. We come now to the most general case. In order to illustrate this case, we start from the Hamiltonian $H=J_x^2 + \kappa^2 J_y^2$. This Hamiltonian reduces to the previous one when $\kappa^2=1$, since then $H=\vec{J}^2 - J_z^2$, which, apart from a constant term, is the same as before. We diagonalize again H in the space of a given irreducible representation, thus obtaining the set of equations

$$H\Psi = E\Psi, \quad C\Psi = j(j+1)\Psi. \tag{9}$$

This set of equations can be connected with a Schrödinger equation with a periodic potential, by realizing the algebra of SU(2), generated by $\vec{J}=\vec{r}\times(-i\nabla)$, in conical coordinates[10] r, θ, φ. These are related to Cartesian coordinates by

$$\begin{aligned} &x=(r/\kappa')\mathrm{dn}\,\theta\,\mathrm{dn}\,\varphi, \quad y=ir(\kappa/\kappa')\mathrm{cn}\,\theta\,\mathrm{cn}\,\varphi, \\ &z=r\kappa\,\mathrm{sn}\,\theta\,\mathrm{sn}\,\varphi, \quad 0\le r<\infty, \quad -2K\le\theta\le 2K, \\ &\mathrm{Re}\,\varphi=K, \quad 0<\mathrm{Im}\,\varphi<2K'. \end{aligned} \tag{10}$$

Here dn, cn, and sn are the Jacobi functions[11] with modulus κ. Furthermore κ' is the complementary modulus, $\kappa^2+\kappa'^2=1$, and $4K$ and $2iK'$ are the real and imaginary periods of $\mathrm{sn}\,\theta$. The generators J_i $(i=x, y, z)$ depend only on the variables θ and φ. These are different from the spherical θ and φ used previously. When written in conical coordinates the Hamiltonian, $H=J_x^2 + \kappa^2 J_y^2$, and Casimir operator, $C=J_x^2+J_y^2+J_z^2$, are given by

$$\begin{aligned} H &= \frac{1}{(\mathrm{sn}^2\theta - \mathrm{sn}^2\varphi)}\left(\mathrm{sn}^2\varphi\frac{\partial^2}{\partial\theta^2} - \mathrm{sn}^2\theta\frac{\partial^2}{\partial\varphi^2}\right), \\ C &= \frac{1}{\kappa^2(\mathrm{sn}^2\theta - \mathrm{sn}^2\varphi)}\left(\frac{\partial^2}{\partial\theta^2} - \frac{\partial^2}{\partial\varphi^2}\right). \end{aligned} \tag{11}$$

The solutions of the set of equations (9) are of the form $\Psi(\theta,\varphi)=\Theta(\theta)\Phi(\varphi)$. The function $\Theta(\theta)$ satisfies the equation[10]

$$\left(-\frac{d^2}{d\theta^2} + j(j+1)\kappa^2\,\mathrm{sn}^2\theta\right)\Theta(\theta) = E\Theta(\theta), \tag{12}$$

and a similar equation in φ holds for $\Phi(\varphi)$. Equation (12) is just a Schrödinger equation in one dimension with a potential proportional to the square of the Jacobi function sn. Replacing θ by ρ, as before, and writing explicitly the parameter κ, we can rewrite (12) as

$$\left(-\frac{d^2}{d\rho^2} + j(j+1)\kappa^2\,\mathrm{sn}^2(\rho,\kappa)\right)\Theta(\rho) = E\Theta(\rho). \tag{13}$$

This equation is known as the Lamé equation.[11] From the known properties of the Jacobi functions, it is possible to infer the properties of the potential $V(\rho)=j(j+1)\kappa^2\,\mathrm{sn}^2(\rho,\kappa)$. For $0\le\kappa^2<1$, $V(\rho)$ is real with a real period $2K$ and therefore it describes a one-dimensional crystal with lattice constant $a=2K$. The physical eigenstates for such a potential are the Bloch wave functions $\Theta_{n,k}(\rho)=e^{ik\rho}u_{n,k}(\rho)$, where $u_{n,k}(\rho)$ is periodic. The energies of these solutions lie within "allowed" bands labeled by n, and k is the crystal momentum. The solutions obtained from the group representations are single valued on the sphere, so that $\Theta(\rho+4K)=\Theta(\rho)$. This implies that the corresponding Θ is a Bloch solution with $k=(\pi/2K)s$, $s=0, \pm1, \pm2, \ldots$ (in the extending zone scheme). Then values of k are mapped for even s to $k=0$ and for odd s to $k=\pm\pi/2K$ in the Brillouin zone. The group solutions thus belong to the edges of the allowed bands. Since finding the eigenvalues of the group Hamiltonian $H=J_x^2 + \kappa^2 J_y^2$ is relatively simple [it amounts to the diagonalization of a $(2j+1)\times(2j+1)$ matrix], the relation between Eq. (13) and the group SU(2) allows one to calculate in a simple way the band structure of the problem. This is shown in Fig. 1 for $j=3$ as a function of κ^2. Since the total number of states in the jth representation is $2j+1$, the number of bands is $j+1$. Note that the Bloch solutions for $k=0, \pm\pi/a$ are standing waves and they can always be chosen real. In the limit, $\kappa^2 \to 1$, the period $2K\to\infty$ and the potential takes the limiting form $V(\rho)=j(j+1)(1-1/\cosh^2\rho)$ which is the Pöschl-Teller potential discussed above, shifted by a constant. The bands of Eq. (13) degenerate into the j sharp bound states of the Pöschl-Teller potential, Fig. 1. A generalization of the transfer matrix M, Eq. (8), of the Pöschl-Teller potential provides the transfer

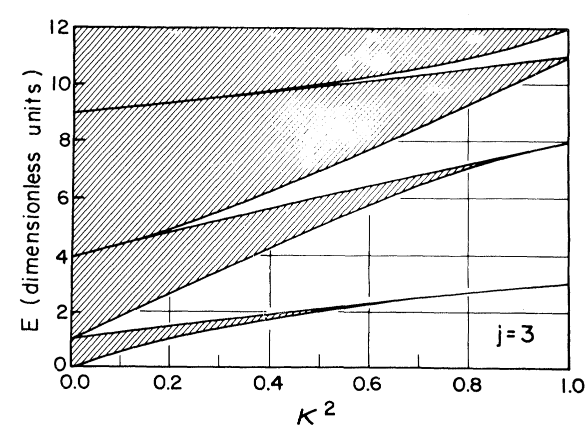

FIG. 1. Band structure of Eq. (13) as a function of the parameter κ^2. The uppermost band continues up to infinite energy.

matrix of the periodic potential $V(\rho)=j(j+1)\kappa^2 \times \mathrm{sn}^2(\rho, \kappa)$. This transfer matrix is still a SU(1, 1) matrix.

In conclusion, the examples discussed in this paper suggest that an algebraic treatment of scattering problems and crystal band structures similar to that of bound-state problems may be possible, and that closed forms for scattering and transfer matrices can be obtained when a dynamical symmetry arises. A detailed presentation of the group-theory approach to scattering in one dimension, including other families of solvable potentials associated with a group, such as the Morse potential (extensively used in molecular physics), can be found in Ref. 12. Our ultimate aim is to apply the group-theoretical description of scattering to atom-atom and nucleus-nucleus collisions.

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