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Multi-state complex angular momentum residues

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Abstract
A relation between a multi-state complex angular momentum (CAM) pole residue and the corresponding CAM-state wavefunction is derived for a real symmetric potential matrix. The result generalizes a residue formula available for single-channel atomical collision systems and it is based on a diagonalization of the S matrix together with the use of exact Wronskian relations.

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1. Introduction

There has been a renewed interest in the complex angular momentum (CAM) approach to analysing elastic and inelastic scattering of atoms and molecules [1–6]. Several numerical methods for locating the CAM (Regge) poles and for determining the pole residues have been developed over the past four decades (see references in [6]). Some of these methods, e.g. the direct Schrödinger method [7], the eigenvalue moment method [8] and the complex absorbing potential technique [1] utilize a particular quadrature formula for determining the pole residues based on the corresponding CAM-state wavefunction. Such a formula is presently available only for single-channel scattering, obtained originally by Newton [9] and recently re-derived by Sokolovski *et al* [1].

Following [1] the single-channel radial Schrödinger equation is given by

$$\frac{d^2\psi_\ell(r)}{dr^2} + \left(k^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\right)\psi_\ell(r) = 0, \tag{1}$$

where k is the asymptotic wave number, ℓ is the angular momentum quantum number and $U(r)$ is the reduced potential that vanishes as $r \to +\infty$. The regular scattering solution can be normalized as

$$\psi_\ell(r) \sim -S_\ell^{-1}\exp(-\mathrm{i}kr + \mathrm{i}\pi\ell/2) + \exp(\mathrm{i}kr - \mathrm{i}\pi\ell/2), \qquad \text{as} \quad r \to +\infty, \tag{2}$$

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where S_ℓ is the S-matrix element. Near the nth CAM pole, ℓ_n, one has $S_\ell \sim \rho_n/(\ell - \ell_n)$ with ρ_n being the pole residue, so that the CAM-state wavefunction $\psi_n(r)$ becomes

$$\psi_n(r) \sim \exp(\mathrm{i}kr - \mathrm{i}\pi\ell_n/2), \qquad \text{as} \quad r \to +\infty. \tag{3}$$

The single-channel residue is then obtained by the formula (see [1])

$$\rho_n = \frac{\mathrm{i}k}{\ell_n + \frac{1}{2}} \left(\int_0^\infty \psi_n^2(r) r^{-2}\,\mathrm{d}r \right)^{-1}, \qquad n = 1, 2, \ldots. \tag{4}$$

In the present work a generalization of (4) to coupled spherically symmetric scattering states is derived. In section 2 an important Wronskian relation that contains information about the multichannel residues is derived. Section 3 discusses general properties of the residue matrix. The final residue formula is obtained in section 4 and conclusions are given in section 5.

2. General Wronskian relations

Consider the matrix version of the radial Schrödinger equation [6]:

$$\frac{\mathrm{d}^2\mathbf{\Psi}_\ell(r)}{\mathrm{d}r^2} + \mathbf{K}_\ell^2(r)\mathbf{\Psi}_\ell(r) = \mathbf{0}, \tag{5}$$

where with the use of the Kronecker delta symbol δ_{ij},

$$\left[\mathbf{K}_\ell^2(r)\right]_{ij} = \delta_{ij}\left(k_j^2 - \ell(\ell+1)/r^2\right) - U_{ij}(r). \tag{6}$$

Here the reduced potential matrix $U_{ij}(r)$ is symmetric and $U_{ij}(r) \to 0$, as $r \to +\infty$. The regular matrix wavefunction may be normalized to satisfy the boundary conditions:

$$\mathbf{\Psi}_\ell(0) = 0, \tag{7}$$

$$\mathbf{\Psi}_\ell(r) \sim -\mathbf{e}_\ell^{(-)}(r)\mathbf{S}_\ell^{-1} + \mathbf{e}_\ell^{(+)}(r), \qquad \text{as} \quad r \to +\infty, \tag{8}$$

with $\mathbf{S}_\ell$ being the S matrix and where the diagonal in- and outgoing, propagating waves $\mathbf{e}_\ell^{(\pm)}(r)$ are given by

$$\left[\mathbf{e}_\ell^{(\pm)}(r)\right]_{ij} = \delta_{ij} k_j^{-1/2}\, \mathrm{e}^{\pm\mathrm{i}(k_j r - \pi\ell/2)}. \tag{9}$$

Note that the amplitudes of the asymptotic waves here are modified by the wave numbers k_j compared to the normalization in (2) and (3).

To proceed, consider the transposed regular solution satisfying

$$\frac{\mathrm{d}^2\mathbf{\Psi}_\ell^T(r)}{\mathrm{d}r^2} + \mathbf{\Psi}_\ell^T(r)\mathbf{K}_\ell^2(r) = \mathbf{0} \tag{10}$$

with the boundary conditions

$$\mathbf{\Psi}_\ell^T(0) = 0, \tag{11}$$

$$[\mathbf{\Psi}_\ell(r)]^T \sim -\left[\mathbf{S}_\ell^{-1}\right]^T \mathbf{e}_\ell^{(-)}(r) + \mathbf{e}_\ell^{(+)}(r), \qquad \text{as} \quad r \to +\infty, \tag{12}$$

and consider also the related solution $\tilde{\mathbf{\Psi}}_\ell(r) \equiv \partial\mathbf{\Psi}_\ell(r)/\partial\ell$ satisfying

$$\frac{\mathrm{d}^2\tilde{\mathbf{\Psi}}_\ell(r)}{\mathrm{d}r^2} + \mathbf{K}_\ell^2(r)\tilde{\mathbf{\Psi}}_\ell(r) = \frac{2\ell+1}{r^2}\mathbf{\Psi}_\ell(r) \tag{13}$$

with the boundary conditions

$$\tilde{\boldsymbol{\Psi}}_\ell(0) = 0, \tag{14}$$

$$\tilde{\boldsymbol{\Psi}}_\ell(r) \sim -\mathbf{e}_\ell^{(-)}(r)\left[\mathrm{i}\frac{\pi}{2}\mathbf{S}_\ell^{-1} + \frac{\partial \mathbf{S}_\ell^{-1}}{\partial \ell}\right] - \mathrm{i}\frac{\pi}{2}\mathbf{e}_\ell^{(+)}(r), \qquad \text{as} \quad r \to +\infty. \tag{15}$$

From the differential equations (5), (10) and (13) one obtains the two Wronskian relations

$$\mathrm{d}\mathbf{W}\big(\boldsymbol{\Psi}_\ell^T, \boldsymbol{\Psi}_\ell\big)/\mathrm{d}r = \mathbf{0}, \tag{16}$$

$$\mathrm{d}\mathbf{W}\big(\boldsymbol{\Psi}_\ell^T, \tilde{\boldsymbol{\Psi}}_\ell\big)/\mathrm{d}r = \frac{2\ell+1}{r^2}\boldsymbol{\Psi}_\ell^T\boldsymbol{\Psi}_\ell, \tag{17}$$

with the Wronskian defined as $\mathbf{W}(\mathbf{X}, \mathbf{Y}) = \mathbf{X}\frac{\mathrm{d}\mathbf{Y}}{\mathrm{d}r} - \frac{\mathrm{d}\mathbf{X}}{\mathrm{d}r}\mathbf{Y}$. Since $\boldsymbol{\Psi}_\ell$, $\boldsymbol{\Psi}_\ell^T$ and $\tilde{\boldsymbol{\Psi}}_\ell$ vanish at the origin one obtains from (16) and (17) the following results:

$$\mathbf{W}\big(\boldsymbol{\Psi}_\ell^T, \boldsymbol{\Psi}_\ell\big) = \mathbf{0}, \tag{18}$$

$$\mathbf{W}\big(\boldsymbol{\Psi}_\ell^T, \tilde{\boldsymbol{\Psi}}_\ell\big)(+\infty) = \int_0^{+\infty} \frac{2\ell+1}{r^2}\boldsymbol{\Psi}_\ell^T(r)\Psi_\ell(r)\,\mathrm{d}r. \tag{19}$$

A study of the analytic forms of the solutions $\Psi_\ell(r)$ and $\boldsymbol{\Psi}_\ell^T(r)$ as $r \to +\infty$ gives

$$\mathbf{W}\big(\boldsymbol{\Psi}_\ell^T, \boldsymbol{\Psi}_\ell\big) = 2\mathrm{i}\big(\mathbf{S}_\ell^{-1} - \big[\mathbf{S}_\ell^{-1}\big]^T\big), \tag{20}$$

which together with (18) implies the symmetry

$$\mathbf{S}_\ell = [\mathbf{S}_\ell]^T. \tag{21}$$

Using the expressions in (12) and (15) together with the symmetry (21), one also obtains

$$\mathbf{W}\big(\boldsymbol{\Psi}_\ell^T, \tilde{\boldsymbol{\Psi}}_\ell\big)(+\infty) = 2\mathrm{i}\frac{\partial \mathbf{S}_\ell^{-1}}{\partial \ell} - 2\pi\mathbf{S}_\ell^{-1}. \tag{22}$$

Equations (19) and (22) yield

$$2\mathrm{i}\frac{\partial \mathbf{S}_\ell^{-1}}{\partial \ell} - 2\pi\mathbf{S}_\ell^{-1} = \int_0^{+\infty} \frac{2\ell+1}{r^2}\boldsymbol{\Psi}_\ell^T(r)\boldsymbol{\Psi}_\ell(r)\,\mathrm{d}r. \tag{23}$$

In the following section we sort out the residue information from the general result (23).

3. Properties of the residue matrix

Sufficiently near the nth CAM pole corresponding to a given channel 'm' one may write the S matrix as

$$\mathbf{S}_\ell \sim \frac{\mathbf{R}_n^{(m)}}{\ell - \ell_n^{(m)}}, \tag{24}$$

where $\mathbf{R}_n^{(m)}$ is the residue matrix at the pole and considered to be independent of ℓ. In case there is a complete de-coupling between the different channels the CAM poles occur in one diagonal S-matrix element only, while the other elements stay finite. It is clear that the residue elements corresponding to the finite S-matrix elements will vanish. In fact, all but one element in $\mathbf{R}_n^{(m)}$ are zero in the de-coupled case. The residue matrix $\mathbf{R}_n^{(m)}$ is also in the general case a singular matrix of rank 1 (see Gell-Mann or Charap and Squires in [11]). This means that even if, generally, all S-matrix elements actually have poles, there exists a particular, complex-valued similarity transformation of $\mathbf{S}_\ell$ to its diagonal form where only one element has a pole.

To analyse the residue matrix in more detail one assumes $\mathbf{S}_\ell$ is symmetric with respect to transposition (see equation (21)). Since $\mathbf{S}_\ell$ also has complex-valued elements it can be represented in the form

$$\mathbf{S}_\ell = \mathbf{O}\mathbf{s}_\ell\,\mathbf{O}^T, \tag{25}$$

where $\mathbf{O}$ is an orthogonal (orthonormal), *complex-valued* matrix and $\mathbf{s}_\ell$ is the *complex* diagonalized S matrix. This statement requires that the columns $\mathbf{o}_m$ of $\mathbf{O}$ are the orthonormal eigenvectors of the S matrix corresponding to the eigenvalues, $s_\ell^{(m)}$, defining the elements of the diagonal matrix $\mathbf{s}_\ell$. In fact, the eigenvalue equations $\mathbf{S}_\ell\mathbf{o}_m = s_\ell^{(m)}\mathbf{o}_m$ and their transposed counterparts, distinguished by substituting $m \to m'$, can be combined to the scalar identities

$$0 = \left(s_\ell^{(m)} - s_\ell^{(m')}\right)\mathbf{o}_{m'}^T\mathbf{o}_m. \tag{26}$$

From (26) one deduces the existence of *orthonormal* columns of $\mathbf{O}$ implying the property $\mathbf{O}^{-1} \equiv \mathbf{O}^T$. Each diagonal element of $\mathbf{s}_\ell$ thus represents an 'eigenchannel' S-matrix element and any CAM pole position $\ell = \ell_n^{(m)}$ corresponds to a unique combination of a pole number 'n' and an eigenchannel 'm', unless there is a so-called channel degeneracy. Now, writing the diagonalized S matrix near an arbitrary CAM pole as

$$\mathbf{s}_\ell \sim \frac{\boldsymbol{\rho}_n^{(m)}}{\ell - \ell_n^{(m)}}, \qquad \ell \to \ell_n^{(m)}, \tag{27}$$

the diagonal matrix $\boldsymbol{\rho}_n^{(m)}$ contains only one non-vanishing element in the mth diagonal position. According to (25) the complete residue matrix is obtained from the formula

$$\mathbf{R}_n^{(m)} = \mathbf{O}\boldsymbol{\rho}_n^{(m)}\mathbf{O}^T, \tag{28}$$

which clearly shows that $\mathbf{R}_n^{(m)}$ is a highly singular matrix just like $\boldsymbol{\rho}_n^{(m)}$.

It turns out to be advantageous to extract the residues from the inverse $\mathbf{S}_\ell^{-1}$, containing finite elements, rather than from $\mathbf{S}_\ell$. From equation (25) one has

$$\mathbf{S}_\ell^{-1} = \mathbf{O}\mathbf{s}_\ell^{-1}\mathbf{O}^T. \tag{29}$$

In fact, the matrix $\mathbf{O}$ should be determined from relation (29) in the first place. The complex angular momentum pole condition is now conveniently written as

$$\det \mathbf{S}_\ell^{-1} = \det \mathbf{s}_\ell^{-1} = 0. \tag{30}$$

In $\mathbf{s}_\ell^{-1}$ one element, say $\left(s_\ell^{(m)}\right)^{-1}$, vanishes at a CAM pole, the others stay nonzero and finite. This vanishing element corresponds to a zero eigenvalue of $\mathbf{S}_\ell^{-1}$ as $\ell \to \ell_n^{(m)}$ and it has information about the pole residue, the others do not. If $\mathbf{o}_m$ is the eigenvector corresponding to the eigenvalue $\left(s_\ell^{(m)}\right)^{-1}$, then

$$\left[\mathbf{S}_\ell^{-1}\mathbf{o}_m\right]_{\ell=\ell_n^{(m)}} = \mathbf{0}. \tag{31}$$

By two inner multiplications of equation (29) with the eigenvector $\mathbf{o}_m$, it is possible to single out the vanishing eigen-channel element. Hence, near a CAM pole

$$\left(s_\ell^{(m)}\right)^{-1} \equiv \left[\mathbf{s}_\ell^{-1}\right]_{mm} = \mathbf{o}_m^T\mathbf{S}_\ell^{-1}\mathbf{o}_m \sim \left(\ell - \ell_n^{(m)}\right)\left(\rho_n^{(m)}\right)^{-1}, \qquad \text{as} \quad \ell \to \ell_n^{(m)}. \tag{32}$$

In this formula the pole residue $\rho_n^{(m)}$ is independent of ℓ, but $\mathbf{S}_\ell^{-1}$ and $\mathbf{o}_m$ are not. By differentiating (32) with respect to ℓ, one obtains after simplifications the relation

$$\rho_n^{(m)} = \left(\mathbf{o}_m^T\frac{\partial\mathbf{S}_\ell^{-1}}{\partial\ell}\mathbf{o}_m\right)^{-1}_{\ell=\ell_n^{(m)}}, \tag{33}$$

since $\mathbf{o}_m$ is an eigenvector of the channel 'm' corresponding to the zero eigenvalue of $\mathbf{S}_\ell^{-1}$. The single, scalar quantity (33) is the only nonzero element of the diagonal residue matrix $\boldsymbol{\rho}_n^{(m)}$, and by (28) it is an important factor of the final residue matrix $\mathbf{R}_n^{(m)}$. When also the individual elements of the matrix $\mathbf{O}$ are introduced one has

$$\left[\mathbf{R}_n^{(m)}\right]_{ij} = \rho_n^{(m)} O_{im} O_{jm}. \tag{34}$$

Formula (34) reveals the simple structure of the multi-state CAM residues that in the 1960s was discussed in more abstract terms [11]: each channel 'm' has a so-called *string* of CAM poles counted by the number 'n'; each such CAM pole defines a matrix of residues determined by the elements of the mth column, $\mathbf{o}_m$, of the matrix $\mathbf{O}$.

4. Residues obtained from the CAM-state wavefunction

According to formulae (23), (31), (33) and (34) one obtains a relation between a residue and the corresponding eigenchannel CAM-state column wavefunction in the form

$$\rho_n^{(m)} = \frac{\mathrm{i}}{\ell_n^{(m)} + 1/2} \left(\int_0^{+\infty} \left[\psi_n^{(m)}(r)\right]^T \psi_n^{(m)}(r) r^{-2}\, \mathrm{d}r \right)^{-1}, \tag{35}$$

where the eigenchannel CAM-state wavefunction $\psi_n^{(m)}(r)$ is defined by

$$\psi_n^{(m)}(r) = \boldsymbol{\Psi}_{\ell_n^{(m)}}(r)\mathbf{o}_m. \tag{36}$$

Formula (35) depends on the normalization of the wavefunction $\boldsymbol{\Psi}_\ell(r)$, which determines the normalization of both $\boldsymbol{\Psi}_\ell^T(r)$ and $\tilde{\boldsymbol{\Psi}}_\ell(r)$. The column wavefunction $\psi_n^{(m)}(r)$ satisfies

$$\psi_n^{(m)}(r) \sim \mathbf{e}_\ell^{(+)}(r)\mathbf{o}_m, \qquad \text{as} \quad r \to +\infty \quad \text{and} \quad \ell \to \ell_n^{(m)}, \tag{37}$$

i.e. it contains no incoming wave components as $r \to +\infty$.

Finally, since (35) determines the single nonzero element in the diagonal residue matrix $\boldsymbol{\rho}_n^{(m)}$, formula (34) provides the complete residue matrix for the original problem.

5. Conclusion

An exact multi-channel formula for calculating CAM pole residues is derived from certain Wronskian relations involving the regular Schrödinger matrix solution and its partial derivative with respect to the complex angular momentum. The formula also involves an orthogonal complex-valued matrix that can always be determined numerically.

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