

Degeneracy of Resonances, Jordan Blocks, and Gamow–Jordan Eigenfunctions

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Received June 30, 2003

We show that a degeneracy of resonances is associated with a second rank pole in the scattering matrix and a Jordan chain of generalized eigenfunctions of the radial Schrödinger equation. The generalized Gamow–Jordan eigenfunctions are basis elements of an expansion in complex resonance energy eigenfunctions. In this biorthonormal basis, any operator $f(H_r^{(\ell)})$ which is a regular function of the Hamiltonian is represented by a nondiagonal complex matrix with a Jordan block of rank 2.

KEY WORDS: nonrelativistic scattering theory; degeneracy of resonances; Berry phase.

1. INTRODUCTION

In recent years there has been an increasing interest in the interference effects in isolated doublets of unbound states and the occurrence of double poles of the scattering matrix. Some interesting examples of interfering unbound two-level systems are the $T = 1$, $T = 0$, $J^\pi = 2^+$ doublet in ^8Be (Hernández and Mondragón, 1994; Hinterberger *et al.*, 1978; von Brentano, 1996), the $T = 1$, $T = 0$ doublet of ρ and ω mesons and the σ - K_s doublet of neutral sigma and K mesons (Baskov *et al.*, 1985; von Brentano, 1994, 1996, 2002; von Brentano *et al.*, 2000). Several, widely differing systems where double poles can occur have been identified, such as autoionizing states in complex atoms Latinne *et al.* (1995) and atomic states in intense laser fields (Kylstra and Joachain, 1998; Magunov *et al.*, 2001). The problem of the degeneracy of resonances also arises naturally in connection with the Berry phase of resonant states (Hernández *et al.*, 1992; Mondragón and Hernández, 1996, 1998; Pont *et al.*, 1992) which was recently measured by the Darmstadt group (Dembowski *et al.*, 2001). Some examples of

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simple quantum mechanical systems with double poles in the scattering matrix have been recently described. Vanroose *et al.* (1997), examined the formation of complex double poles of the S -matrix in a two-channel model with square well potentials. Recently, Hernández *et al.* (2000), investigated a one-channel model with two spherical concentric cavities bounded by δ -function barriers and showed that a double pole of the S -matrix can be induced by tuning the parameters of the model; Vanroose generalized this model to the case of two finite width barriers (Vanroose, 2001). The formal theory of multiple pole resonances and resonant states in the rigged Hilbert space formulation of quantum mechanics was developed by Bohm *et al.* (1997), and by Antoniou *et al.* (1998).

In the present paper, we deal with the problem of multiple poles of the scattering matrix and the generalized complex energy eigenfunctions associated with them in the framework of the theory of the analytic properties of the radial wave functions.

The plan of this paper is as follows. In Section 2, we introduce some basic concepts and fix the notation by way of a short reminder of resonances and resonant states in the theory of the analytic properties of the radial wave functions. Sections 3 and 4 are devoted to a short discussion of the no-crossing rule for bound states and its nonapplicability to resonant states. In Section 5, we show that a double pole of the Green's function (double zero of the Jost function) is associated with a chain of length two of Gamow–Jordan generalized eigenfunctions and derive explicit expressions for this generalized eigenfunctions in terms of the outgoing wave Jost solution, the Jost function and its derivatives evaluated at the double pole. We give the normalization and orthogonality rules for the generalized eigenfunctions in the Jordan chain associated to the double pole of the Green's function in Section 6. Section 7 is devoted to showing that the Gamow–Jordan generalized eigenfunctions in the Jordan chain are elements of a complete set of states containing the real (bound states) and complex (resonant state) energy eigenfunctions plus a continuum of scattering wave functions of complex wave number. In Section 8 we derive expansion theorems (spectral representations) for operators $f(H_r^{(\ell)})$ which are regular functions of the radial Hamiltonian $H_r^{(\ell)}$ and show that, in this basis, the operator $f(H_r^{(\ell)})$ is represented by a complex matrix which is diagonal except for a Jordan block of rank 2 associated to the double zero of the Jost function and the corresponding Jordan chain of generalized Gamow–Jordan eigenfunction. We end our paper with a summary of results and some conclusions in Section 9.

2. REGULAR AND PHYSICAL SOLUTIONS OF THE RADIAL EQUATION

The nonrelativistic scattering of a spinless particle by a short ranged potential $v(r)$ is described by the solution of a Schrödinger equation. When the potential is rotationally invariant, the wave function is expanded in partial waves and one is

left with the radial equation

$$\frac{d^2\phi_\ell(k, r)}{dr^2} + \left[k^2 - \frac{\ell(\ell + 1)}{r^2} - v(r) \right] \phi_\ell(k, r) = 0. \tag{1}$$

As is usually done when discussing the analytic properties of the solutions of (1) as functions of k , rather than starting by defining the physical solutions $\psi_\ell^{(+)}(k, r)$, we define the regular and irregular solutions of (1) by boundary conditions which lead to simple properties as functions of k . The regular solution $\phi_\ell(k, r)$ is uniquely defined by the boundary condition (Newton, 1982)

$$\lim_{r \rightarrow 0} (2\ell + 1)!! r^{-\ell-1} \phi_\ell(k, r) = 1, \tag{2}$$

$\phi_\ell(k, r)$ may be expressed as a linear combination of two independent, irregular solutions of (1) which behave as outgoing and incoming waves at infinity,

$$\phi_\ell(k, r) = \frac{1}{2} i k^{-\ell-1} [f_\ell(-k) f_\ell(k, r) - (-1)^\ell f_\ell(k) f_\ell(-k, r)], \tag{3}$$

where $f_\ell(-k, r)$ is an outgoing wave at infinity defined by the boundary condition

$$\lim_{r \rightarrow \infty} \exp(-ikr) f_\ell(-k, r) = (+i)^\ell \tag{4}$$

and $f_\ell(k, r)$ is an incoming wave at infinity related to $f_\ell(-k, r)$ by

$$f_\ell(k, r) = (-1)^\ell f_\ell^*(-k, r) \tag{5}$$

for k real and nonvanishing.

The Jost function $f_\ell(-k) = f_\ell(-k, 0)$ is given by

$$f_\ell(-k) = (-1)^\ell k^\ell W[f_\ell(-k, r), \phi_\ell(k, r)], \tag{6}$$

where $W[f, g] = fg' - f'g$ is the Wronskian. The Jost function $f_\ell(-k)$, has zeroes (roots) on the imaginary axis and in the lower half of the complex k -plane.

When the first and second absolute moments of the potential exist, and the potential decreases at infinity faster than any exponential (e.g., if $v(r)$ has a Gaussian tail or if it vanishes identically beyond a finite radius) the functions $f_\ell(-k)$, $\phi_\ell(k, r)$, and $k^\ell f_\ell(-k, r)$, for fixed $r > 0$, are entire functions of k (Newton, 1982).

Therefore, the derivatives of these functions with respect to the wave number k exist and are entire functions of k for all finite values of k in the complex k -plane.

The differential equations satisfied by the derivatives of the functions $\phi_\ell(k, r)$ and $f_\ell(-k, r)$ with respect to k are obtained from (1) taking derivatives with respect to k on both sides of the equation,

$$\frac{d^2\dot{\phi}_\ell(k, r)}{dr^2} + \left[k^2 - \frac{\ell(\ell + 1)}{r^2} - v(r) \right] \dot{\phi}_\ell(k, r) = -2k\phi_\ell(k, r), \tag{7}$$

$$\frac{d^2\ddot{\phi}_\ell(k, r)}{dr^2} + \left[k^2 - \frac{\ell(\ell + 1)}{r^2} - v(r) \right] \ddot{\phi}_\ell(k, r) = -4k\dot{\phi}_\ell(k, r) - 2\phi_\ell(k, r), \tag{8}$$

in (7) and (8) we have used the notation $\dot{\phi}_\ell(k, r) = d\phi_\ell(k, r)/dk$. Similar expressions are valid for the derivatives with respect to k of the outgoing wave solutions $f_\ell(-k, r)$.

The scattering wave function $\psi_\ell^{(+)}(k, r)$ is the solution of Eq. (1) which vanishes at the origin and behaves at infinity as the sum of a free incoming spherical wave of unit incoming flux plus a free outgoing spherical wave,

$$\psi_\ell^{(+)}(k, 0) = 0 \tag{9}$$

and

$$\lim_{r \rightarrow \infty} \{ \psi_\ell^{(+)}(k, r) - [\hat{h}_\ell^{(-)}(k, r) - S_\ell(k)\hat{h}_\ell^{(+)}(k, r)] \} = 0. \tag{10}$$

In this expression $\hat{h}_\ell^{(-)}(k, r)$ and $\hat{h}_\ell^{(+)}(k, r)$ are Ricatti–Hankel functions that describe incoming and outgoing waves respectively, $S_\ell(k)$ is the scattering matrix.

Hence, the scattering wave function $\psi_\ell^{(+)}(k, r)$ and the regular solution are related by

$$\psi_\ell^{(+)}(k, r) = \frac{k^{\ell+1}\phi_\ell(k, r)}{f_\ell(-k)}, \tag{11}$$

and the scattering matrix is given by

$$S_\ell(k) = \frac{f_\ell(k)}{f_\ell(-k)}. \tag{12}$$

The complete Green’s function for outgoing particles or resolvent of the radial equation may also be written in terms of the regular solution $\phi_\ell(k, r)$ and the irregular solution $f_\ell(-k, r)$ which behaves as an outgoing wave at infinity

$$G_\ell^{(+)}(k; r, r') = (-1)^{\ell+1} k^\ell \frac{\phi_\ell(k, r_<)f_\ell(-k, r_>)}{f_\ell(-k)}. \tag{13}$$

3. BOUND AND RESONANT STATE EIGENFUNCTIONS

Bound and resonant state energy eigenfunctions are the solutions of (1) which vanish at the origin

$$u_{n\ell}(k_n, 0) = 0, \tag{14}$$

and at infinity satisfy the boundary condition

$$\lim_{r \rightarrow \infty} \left[\frac{1}{u_{n\ell}(k_n, r)} \frac{du_{n\ell}(k_n, r)}{dr} - ik_n \right] = 0, \tag{15}$$

where k_n is a zero of the Jost function,

$$f_\ell(-k_n) = 0. \tag{16}$$

From Eqs. (1) and (3) we verify that all roots (zeroes) of the Jost function are associated to energy eigenfunctions of the Schrödinger equation.

Bound state eigenfunctions are associated to the zeroes of $f_\ell(-k)$ which lay on the positive imaginary axis $k_s^2 = -\kappa_s^2 < 0$, while resonant or Gamow state eigenfunctions are associated to the zeroes of the Jost function which lay in the fourth quadrant of the complex κ -plane.

From (3), (4), and (16), bound states and Gamow or resonance eigenfunctions are related to the regular solution $\phi_\ell(k, r)$ by

$$u_{n\ell}(k_n, r) = N_{n\ell}^{-1} \phi_\ell(k_n, r), \tag{17}$$

where $N_{n\ell}$ is a normalization constant. Because of the vanishing of $f_\ell(-k_n)$, $\phi_\ell(k_n, r)$, is now proportional to the outgoing wave solution, $f_\ell(-k_n, r)$, of (1). Hence,

$$u_{n\ell}(k_n, r) = N_{n\ell}^{-1} \frac{i (-i)^{\ell+1}}{2 k^{\ell+1}} f_\ell(k_n) f_\ell(-k_n, r). \tag{18}$$

This expression shows, in a very explicit way, that the Gamow state eigenfunctions $u_{n\ell}(k_n, r)$ with $k_n = \kappa_n - i\gamma_n$ and $\kappa_n > \gamma_n > 0$, are solutions of (1) which vanish at the origin and asymptotically behave as purely outgoing waves which oscillate between envelopes that increase exponentially with r , the corresponding energy eigenvalues \mathcal{E}_n are complex with $\Re(\mathcal{E}_n) > \Im(\mathcal{E}_n)$.

The bound state eigenfunctions $u_{s\ell}(k_s, r)$ are also solutions of (1) which satisfy the boundary conditions (14) and (15), but, in this case, $k_s = i\kappa_s$ with, $\kappa_s > 0$, which means that asymptotically the outgoing wave of imaginary argument, $f_\ell(-k_s, r)$, decreases exponentially with r and the energy eigenvalue \mathcal{E}_s is real and negative.

4. THE NO-CROSSING RULE FOR BOUND STATES

In the case of bound states, the normalization constant is related to the derivative of the Jost function evaluated at k_s and it may also be expressed as a normalization integral. The zero of the Jost function is on the positive imaginary axis, and the bound state eigenfunction is quadratically integrable (for time reversal invariant forces $\phi_\ell(i\kappa_s, r)$ is real). Newton (1982) gives the following expression:

$$N_{s\ell}^2 = \frac{1}{i4k_s^{2(\ell+1)}} \left(\frac{df_\ell(-k)}{dk} \right)_{k_s} f_\ell(k_s) = \int_0^\infty |\phi_\ell(k_s, r)|^2 dr. \tag{19}$$

Since the normalization integral is positive and the function $f_\ell(k)$ is regular at $k_s = i\kappa_s$, the derivative of the Jost function evaluated at $k_s = i\kappa_s$ cannot vanish. Therefore, the zero of $f_\ell(-k)$ at $k_s = i\kappa_s$ must be simple. The corresponding pole in $G_\ell^{(+)}(k; r, r')$, $\psi_\ell^{(+)}(k, r)$, and $S_\ell(k)$ must also be simple.

It follows that, in the absence of symmetry, the real, negative energy eigenvalues of the radial equation for a one-channel problem cannot be degenerate.

5. THE NO-CROSSING RULE DOES NOT HOLD FOR RESONANCE STATES

In the case of a resonant state, the zero of the Jost function $f_\ell(-k)$ lies in the fourth quadrant of the complex k -plane,

$$k_n = \kappa_n - i\gamma_n, \tag{20}$$

with $k_n > \gamma_n > 0$.

The resonant or Gamow eigenfunction $\phi_\ell(k_n, r)$ is an outgoing spherical wave of complex wave number k_n and angular momentum ℓ . Therefore, for large values of r , $\phi_\ell(k_n, r)$ oscillates between envelopes that grow exponentially with r . Hence, the integrals over r must be properly defined. This may be done by means of a Gaussian regulator and a limiting procedure (Zel'dovich, 1960, 1961). Berggren (1968, 1996) gives the following expression:

$$\frac{1}{i4k_n^{2(\ell+1)}} \left(\frac{df_\ell(-k)}{dk} \right)_{k_n} f_\ell(k_n) = \lim_{\nu \rightarrow 0} \int_0^\infty \exp(-\nu r^2) \phi_\ell^2(k_n, r) dr \tag{21}$$

The integral on the right-hand side is a complex number and it may vanish.

Since $f_\ell(k_n)$ has no zeroes in the lower half of the complex k -plane, the left-hand side of Eq. (21) vanishes only when $(df_\ell(-k)/dk)_{k_n}$ vanishes. Then, we have two possibilities:

- (i) When $(df_\ell(-k)/dk)_{k_n}$ does not vanish, $f(-k)$, has a simple zero at $k = k_n$, the integral on the right-hand side of Eq. (21) does not vanish and the normalization constant, $N_{n\ell}^2$, occurring in (17) is given by (21).
- (ii) When

$$\left(\frac{df_\ell(-k)}{dk} \right)_{k_n} = 0, \tag{22}$$

the integral on the right-hand side of (21) vanishes,

$$\lim_{\nu \rightarrow 0} \int_0^\infty \exp(-\nu r^2) \phi_\ell^2(k_n, r) dr = 0 \tag{23}$$

and the Jost function $f_\ell(-k)$ has a multiple zero at $k = k_n$. In this case, the Green's function $G_\ell^{(+)}(k; r, r')$, the scattering wave function, $\psi_\ell^{(+)}(k, r)$ and the scattering matrix $S_\ell(k)$ have a multiple pole at $k = k_n$. The normalization constant of the Gamow eigenfunction is no longer given by (21).

Furthermore, it will be shown below that when $f_\ell(-k)$ has a multiple zero (a multiple resonant pole of rank r in $G_\ell^{(+)}(k; r, r')$, $\psi_\ell^{(+)}(k, r)$, and $S_\ell(k)$) the corresponding complex energy eigenvalues are degenerate even in the absence of symmetry. That is, the no-crossing rule does not hold for resonant eigenstates.

6. DOUBLE POLES IN THE GREEN’S FUNCTION

A convenient way to relate resonant states with processes of physical interest is via the Green’s function or resolvent of the radial equation with outgoing wave boundary conditions. The spectral representation of the complete Green’s function $G_\ell^{(+)}(k; r, r')$ for outgoing particles is (Newton, 1982)

$$G_\ell^{(+)}(k; r, r') = \sum_{\substack{s \text{ bound} \\ \text{states}}} \frac{v_{s\ell}(k, r)v_{s\ell}^*(k, r')}{k^2 + \kappa_s^2} + \frac{2}{\pi} \int_0^\infty dk' \frac{\psi_\ell^{(+)}(k', r)\psi_\ell^{(+)*}(k', r')}{(k^2 - k'^2)}. \tag{24}$$

In the following it will be assumed that the Jost function $f_\ell(-k')$ has a double resonance zero at $k' = k_m$ in the fourth quadrant of the k' -plane, all other zeroes of $f_\ell(-k')$ in the same quadrant being simple. Then, from (11), the scattering solution $\psi_\ell^{(+)}(k', r)$ as function of k' -complex has one double resonance pole at $k' = k_m$ and simple resonance poles at $k' = k_n, n = 1, 2, \dots, m - 1, m + 1 \dots$, all k_n in the fourth quadrant of the complex k' -plane. The function $\psi_\ell^{(+)*}(k', r')$ is regular in the lower half of the complex k' -plane.

The integration contour in the second term on the right-hand side of (24) may be deformed into the lower half of the complex k' -plane, as shown in Fig. 1. When the deformed contour C crosses over resonant poles, the theorem of the residue gives

$$G_\ell^{(+)}(k; r, r') = \sum_{\substack{s \text{ bound} \\ \text{states}}} \frac{v_{s\ell}(k, r)v_{s\ell}^*(k, r')}{k^2 + \kappa_s^2} + \sum_{\substack{n \text{ resonant} \\ \text{poles}}} 2\pi i \text{Res} \left[\frac{2}{\pi} \frac{\psi_\ell^{(+)}(k', r)\psi_\ell^{(+)*}(k', r')}{(k^2 - k'^2)} \right]_{k'=k_n} + \frac{2}{\pi} \int_C dk' \frac{\psi_\ell^{(+)}(k', r)\psi_\ell^{(+)*}(k', r')}{(k^2 - k'^2)}. \tag{25}$$

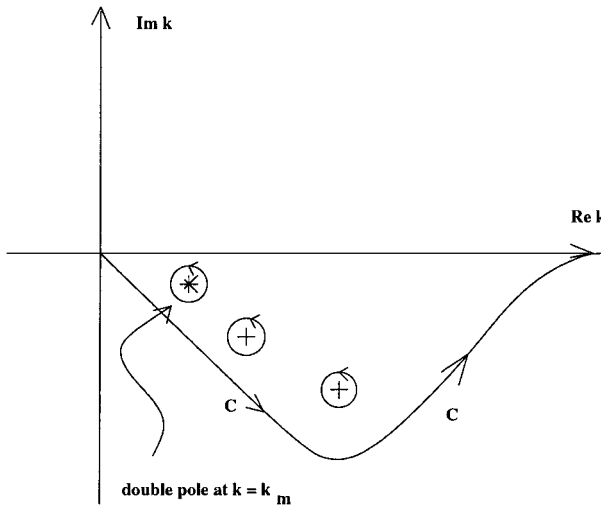


Fig. 1. Integration contour C in the complex k' -plane.

6.1. Residue at a Simple Pole

When $f_\ell(-k')$ has a simple zero at k_n

$$f_\ell(-k') = (k' - k_n)g_{n\ell}(k'). \tag{26}$$

Then, from (3), (5), (11), and (26)

$$\begin{aligned} 2\pi i \text{Res} \left[\frac{2}{\pi} \frac{\psi_\ell^{(+)}(k', r)\psi_\ell^{(+)*}(k', r')}{k^2 - k'^2} \right]_{k'=k_n} \\ = 2\pi i \lim_{k' \rightarrow k_n} \frac{2}{\pi} \left[\frac{\phi_\ell(k', r)\phi_\ell(k', r')k'^{2(\ell+1)}}{g_{n\ell}(k')f_\ell(k')(k^2 - k'^2)} \right], \end{aligned} \tag{27}$$

which may be written as

$$2\pi i \text{Res} \left[\frac{2}{\pi} \frac{\psi_\ell^{(+)}(k', r)\psi_\ell^{(+)*}(k', r')}{(k^2 - k'^2)} \right]_{k'=k_n} = \frac{u_{n\ell}(k_n, r)u_{n\ell}(k_n, r')}{k^2 - k_n^2}, \tag{28}$$

which is the well-known expression that shows that $G_\ell^{(+)}(k; r, r')$ as function of k -complex has a simple pole at $k = k_n$ with residue $u_{n\ell}(k_n, r)u_{n\ell}(k_n, r')$. The Gamow eigenfunction or normal mode, $u_{n\ell}(k_n, r)$, is given by (18) and the normalization constant $N_{n\ell}$ is given by

$$N_{n\ell}^2 = \frac{1}{i4k_n^{2(\ell+1)}} f_\ell(k_n) \left(\frac{df_\ell(-k')}{dk'} \right)_{k_n}, \tag{29}$$

in agreement with Berggren's result given in Eq. (21).

6.2. Residue at a Double Pole

When $f_\ell(-k')$ has a double zero at $k' = k_m$, we may write

$$f_\ell(-k') = (k' - k_m)^2 g_{\ell m}(k') \tag{30}$$

the function $g_{\ell m}(k')$ is regular at $k' = k_m$ and may be expanded as

$$g_{\ell m}(k') = \frac{1}{2} \left(\frac{d^2 f_\ell(-k')}{dk'^2} \right)_{k_m} + \frac{1}{6} (k' - k_m) \left(\frac{d^3 f_\ell(-k')}{dk'^3} \right)_{k_m} + \dots \tag{31}$$

with

$$\left(\frac{d^2 f_\ell(-k')}{dk'^2} \right)_{k_m} \neq 0. \tag{32}$$

Thus, the scattering wave function $\psi_\ell^{(+)}(k', r)$ has a double pole at $k' = k_m$,

$$\psi_\ell^{(+)}(k', r) = \frac{\phi_\ell(k', r) k'^{\ell+1}}{(k' - k_m)^2 g_{\ell m}(k')}, \tag{33}$$

but $\psi_\ell^{(+)*}(k', r')$ is regular at $k' = k_m$, since $f_\ell(k')$ has no zeroes in the lower half of the complex k' -plane,

$$\psi_\ell^{(+)*}(k', r') = \frac{\phi_\ell(k', r') k'^{\ell+1}}{f_\ell(k')}. \tag{34}$$

Then, the residue of the Green’s function $G_\ell^{(+)}(k'; r, r')$ at the double pole in $k' = k_m$ is obtained from the Cauchy integral formula as

$$\begin{aligned} & 2\pi i \operatorname{Res} \left[\frac{2}{\pi} \frac{\psi_\ell^{(+)}(k', r) \psi_\ell^{(+)*}(k', r')}{(k^2 - k'^2)} \right]_{k'=k_m} \\ &= 4i \left\{ \frac{d}{dk'} \left[\frac{\phi_\ell(k', r) \phi_\ell(k', r') k'^{2(\ell+1)}}{g_{\ell m}(k') f_\ell(k') (k^2 - k'^2)} \right] \right\}_{k'=k_m}. \end{aligned} \tag{35}$$

After computing the derivative and rearranging some terms, we obtain

$$\begin{aligned} & 2\pi i \operatorname{Res} \left[\frac{2}{\pi} \frac{\psi_\ell^{(+)}(k', r) \psi_\ell^{(+)*}(k', r')}{(k^2 - k'^2)} \right]_{k'=k_m} \\ &= \frac{1}{\mathcal{N}_{m,\ell}^2} \frac{\hbar^2}{2\mu} \left[\frac{\phi_\ell(k_m, r) \phi_\ell(k_m, r')}{(E - \mathcal{E}_m)^2} \right. \\ & \quad \left. + \frac{\phi_\ell(k_m, r) \hat{\phi}_\ell(k_m, r') + \hat{\phi}_\ell(k_m, r) \phi_\ell(k_m, r')}{(E - \mathcal{E}_m)} \right], \end{aligned} \tag{36}$$

where, according to (17), $\phi_\ell(k_m, r)$ is the nonnormalized Gamow eigenfunction and $\hat{\phi}_\ell(k_m, r)$ is a generalized Gamow–Jordan eigenfunction or abnormal mode given by

$$\hat{\phi}_\ell(k_m, r) = \frac{d\phi_\ell(k_m, r)}{d\mathcal{E}_m} + C_\ell(k_m)\phi_\ell(k_m, r), \tag{37}$$

\mathcal{E}_m is the complex energy eigenvalue, $\mathcal{E}_m = (\hbar^2/2\mu)k_m^2$, and the constant factor $C_\ell(k_m)$, multiplying $\phi_\ell(k_m, r)$ in Eq. (37), is

$$C_\ell(k_m) = \frac{2\mu}{\hbar^2} \frac{1}{2k_m} \left[\frac{\ell + 1}{k_m} - \frac{1}{2} \frac{1}{f_\ell(k_m)} \frac{df_\ell(k_m)}{dk_m} - \frac{1}{6} \left(\frac{d^2 f_\ell(-k')}{dk'^2} \right)_{k_m}^{-1} \left(\frac{d^3 f_\ell(-k')}{dk'^3} \right)_{k_m} \right]. \tag{38}$$

The normalization constant $\mathcal{N}_{m\ell}^2$ is now

$$\mathcal{N}_{m\ell}^2 = \left(\frac{2\mu}{\hbar^2} \right) \frac{1}{16ik_m^{2\ell+3}} f_\ell(k_m) \left(\frac{d^2 f_\ell(-k')}{dk'^2} \right)_{k_m}. \tag{39}$$

The expression (36) suggests the following normalization rule for the chain of Gamow–Jordan generalized eigenfunctions belonging to a double pole of $G_\ell^{(+)}(k', r, r')$

$$u_{m\ell}(k_m, r) = \frac{1}{\mathcal{N}_{m\ell}} \phi_\ell(k_m, r), \tag{40}$$

and

$$\hat{u}_{m\ell}(k_m, r) = \frac{1}{\mathcal{N}_{m\ell}} \hat{\phi}_\ell(k_m, r). \tag{41}$$

Substitution of (40) and (41) in (36) gives

$$\begin{aligned} & 2\pi i \text{Res} \left[\frac{2}{\pi} \frac{\psi_\ell^{(+)}(k', r) \psi_\ell^{(+)*}(k', r')}{(k^2 - k'^2)} \right]_{k'=k_m} \\ &= \frac{\hbar^2}{2\mu} \left[\frac{u_{m\ell}(k_m, r) u_{m\ell}(k_m, r')}{(E - \mathcal{E}_m)^2} + \frac{u_{m\ell}(k_m, r) \hat{u}_{m\ell}(k_m, r') + \hat{u}_{m\ell}(k_m, r) u_{m\ell}(k_m, r')}{(E - \mathcal{E}_m)} \right]. \end{aligned} \tag{42}$$

This result shows that a pole of second order in the Green’s function $G_\ell^{(+)}(k; r, r')$ is associated with a chain of two generalized Gamow–Jordan eigenfunctions, $u_{m,\ell}(k_m, r)$ and $\hat{u}_{m\ell}(k_m, r)$ which belong to the same complex energy eigenvalue $\mathcal{E}_m = (\hbar^2/2\mu)k_m^2$.

Finally, substitution of (28) and (42) in (25) gives the following expression for the complete Green’s function of the radial equation

$$\begin{aligned}
 G_\ell^{(+)}(k; r, r') = & \frac{\hbar^2}{2\mu} \left[\sum_{\substack{s \text{ bound} \\ \text{states}}} \frac{v_{s\ell}(k, r)v_{s\ell}^*(k, r')}{E + |E_s|} \right. \\
 & + \sum_{\substack{n \neq m \\ \text{resonant} \\ \text{states}}} \frac{u_{n\ell}(k_n, r)u_{n\ell}(k_n, r')}{E - \mathcal{E}_n} \\
 & + \frac{u_{m\ell}(k_m, r)u_{m\ell}(k_m, r')}{(E - \mathcal{E}_m)^2} \\
 & \left. + \frac{u_{m\ell}(k_m, r)\hat{u}_{m\ell}(k_m, r') + \hat{u}_{m\ell}(k_m, r)u_{m\ell}(k_m, r')}{(E - \mathcal{E}_m)} \right] \\
 & + \frac{2}{\pi} \int_C \frac{\psi_\ell^{(+)}(k', r)\psi_\ell^{(+)*}(k', r')}{(k^2 - k'^2)} dk'. \tag{43}
 \end{aligned}$$

7. ORTHOGONALITY AND NORMALIZATION INTEGRALS FOR GAMOW–JORDAN EIGENFUNCTION

As in the case of bound and resonant state eigenfunctions associated with simple poles of the Green’s function, we may derive orthogonality and normalization rules for the Gamow–Jordan eigenstates in terms of regularized integrals of the generalized Gamow–Jordan eigenfunctions. Following the same procedure as in Berggren (1968, 1996), it may be shown that, when $f_\ell(-k')$ has a double zero at $k' = k_m$, the following relations are valid,

$$\begin{aligned}
 & \frac{1}{i8k_m^{2(\ell+1)}} f_\ell(k_m) \left(\frac{d^2 f_\ell(-k')}{dk'^2} \right)_{k'=k_m} \\
 & = \lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \frac{d\phi_\ell(k_m, r)}{dk_m} \phi_\ell(k_m, r) dr \tag{44}
 \end{aligned}$$

and

$$\begin{aligned}
 & \frac{1}{i8k_m^{2(\ell+1)}} f_\ell(k_m) \left[\frac{1}{3} \left(\frac{d^3 f_\ell(-k')}{dk'^3} \right)_{k_m} \right. \\
 & \left. - \left(\frac{d^2 f_\ell(-k')}{dk'^2} \right)_{k_m} \left(\frac{2(\ell + 1)}{k_m} - \frac{1}{f_\ell(k_m)} \frac{df_\ell(k_m)}{dk_m} \right) \right]
 \end{aligned}$$

$$= \lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \left(\frac{d\phi_\ell(k_m, r)}{dk_m} \right)^2 dr. \quad (45)$$

From the expression (38) for $C_\ell(k_m)$ and Eqs. (44) and (45), it follows that

$$\begin{aligned} & \lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \left(\frac{d\phi_\ell(k_m, r)}{dk_m} \right)^2 dr + 2C_\ell(k_m) \frac{\hbar^2 k_m}{\mu} \\ & \times \left(\lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \frac{d\phi_\ell(k_m, r)}{dk_m} \phi_\ell(k_m, r) dr \right) = 0, \end{aligned} \quad (46)$$

which may be rewritten as

$$\begin{aligned} & \lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \left[\frac{d\phi_\ell(k_m, r)}{d\mathcal{E}_m} + C_\ell(k_m) \phi_\ell(k_m, r) \right]^2 dr \\ & = C_\ell^2(k_m) \lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \phi_\ell^2(k_m, r) dr, \end{aligned} \quad (47)$$

but, according to Eqs. (22) and (23), when $f_\ell(-k)$ has a double zero at $k = k_m$, the integral on the right-hand side of (47) vanishes. Therefore, the integrand on the left-hand side of (47) is the square of the generalized Jordan-Gamow eigenfunction and the relation (45) translates into

$$\lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \hat{\phi}_\ell^2(k_m, r) dr = 0 \quad (48)$$

which shows that also the regularized integral of the square of the generalized Gamow-Jordan eigenfunction vanishes.

An expression for the normalization constant $\mathcal{N}_{m\ell}^2$ in terms of a normalization integral may be obtained from (44) and (39),

$$\mathcal{N}_{m\ell}^2 = \lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \frac{d\phi_\ell(k_m, r)}{d\mathcal{E}_m} \phi_\ell(k_m, r) dr \quad (49)$$

writing $d\phi_\ell/d\mathcal{E}_m$ in terms of $\hat{\phi}_\ell(k_m, r)$ and recalling that the integral of $\phi_\ell^2(k_m, r)$ vanishes, we get

$$\mathcal{N}_{m\ell}^2 = \lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \hat{\phi}_\ell(k_m, r) \phi_\ell(k_m, r) dr, \quad (50)$$

which shows that the right-hand side of (50) is the normalization integral for the Gamow-Jordan generalized eigenfunctions associated with a double pole degeneracy of resonances. However, it is convenient to note that this expression does not fix the normalization rule for $\phi_\ell(k_m, r)$ and $\hat{\phi}_\ell(k_m, r)$ in a unique way. Since $\phi_\ell(k_m, r)$ and $\hat{\phi}_\ell(k_m, r)$ are linearly independent, they have different dimensions and its product has no obvious interpretation in terms of observable quantities,

therefore, there is no a priori reason to normalize both functions with the same normalization constant. Thus, we still have the freedom to write (50) as

$$\lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \left(\frac{X_m}{\mathcal{N}_{m,\ell}} \hat{\phi}_\ell(k_m, r) \right) \left(\frac{1}{X_m \mathcal{N}_{m,\ell}} \phi_\ell(k_m, r) \right) dr = 1, \tag{51}$$

where $\mathcal{N}_{m,\ell}^2$ is given in (39) and X_m is a non-vanishing real or complex number that we associate with the double pole singularity of $G_\ell^{(+)}(k; r, r')$ at $k = k_m$. Therefore, a more general normalization rule for the Gamow and Gamow–Jordan generalized eigenfunction that the one proposed in (40) and (41) would be

$$u_{m\ell}(k_m, r) = \frac{1}{X_m \mathcal{N}_{m,\ell}} \phi_\ell(k_m, r) \tag{52}$$

and

$$\hat{u}_{m\ell}(k_m, r) = \frac{X_m}{\mathcal{N}_{m,\ell}} \hat{\phi}_\ell(k_m, r). \tag{53}$$

With this normalization, the orthogonality and normalization integrals for the Gamow–Jordan generalized eigenfunction associated to a double pole of the Green’s function, Eqs. (21), (48), and (50) take the form

$$\lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} u_{m,\ell}^2(k_m, r) dr = 0 \tag{54}$$

$$\lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} \hat{u}_{m,\ell}^2(k_m, r) dr = 0 \tag{55}$$

and

$$\lim_{\nu \rightarrow 0} \int_0^\infty e^{-\nu r^2} u_{m,\ell}(k_m, r) \hat{u}_{m,\ell}(k, r) dr = 1 \tag{56}$$

The form of these orthogonality and normalization conditions is independent of the value of the constant X_m . However, if the Gamow–Jordan generalized eigenfunction are normalized according to (52) and (53), the expression for the residue at the double pole of $G_\ell^{(+)}(k; r, r')$ would be explicitly dependent on X_m , since a factor X_m^2 will appear multiplying the term $u_{m\ell}(k_m, r) u_{m\ell}(k_m, r')$ in the expression for the residue at the double pole of $G_\ell^{(+)}(k; r, r')$ given in Eq. (43),

$$\begin{aligned} & \frac{X_m^2 u_{m\ell}(k_m, r) u_{m\ell}(k_m, r')}{(E - \mathcal{E}_m)^2} \\ & + \frac{u_{m\ell}(k_m, r) \hat{u}_{m\ell}(k_m, r') + \hat{u}_{m\ell}(k_m, r) u_{m\ell}(k_m, r')}{(E - \mathcal{E}_m)}. \end{aligned} \tag{57}$$

As is evident from the definition (37), the generalized eigenfunctions $\phi_{n\ell}(k_m, r)$ and $\hat{\phi}_{n\ell}(k_m, r)$ have different dimensions, if one takes X_m of dimension (energy)^{1/2}

the normalized eigenfunctions $u_{n\ell}(k_n, r)$ and $\hat{u}_{n\ell}(k_n, r)$ have the same dimensions namely $(\text{energy})^{-1/2}$ so that when $(X_m) = (\text{energy})^{1/2}$ the higher order Gamow–Jordan vectors become Jordan vectors with the same dimensions as the Gamow vectors.

This freedom in the normalization rules could be used to define normalized Gamow–Jordan eigenfunctions with the same dimensions as those of the Gamow eigenfunctions associated to simple poles of $G_\ell^{(+)}(k; r, r')$.

However, to keep the notation as simple and transparent as possible, in this paper, we will choose $X_m = 1$, and normalize the Gamow–Jordan eigenfunctions according to the rule given in (40) and (41).

8. COMPLETENESS AND THE EXPANSION IN COMPLEX RESONANCE ENERGY EIGENFUNCTIONS

In this section it will be shown that the Gamow–Jordan generalized eigenfunctions are basis elements of an expansion in complex resonance energy eigenfunctions.

Given two square integrable and very well behaved functions $\Phi(r)$ and $\chi(r)$ which decrease at infinity faster than any exponential, the completeness of the orthonormal set of bound state and scattering solutions of the radial Schrödinger equation (Newton, 1982) allows us to write

$$\langle \Phi | \chi \rangle = \sum_{\substack{s \text{ bound} \\ \text{states}}} \langle \Phi | v_{s,\ell} \rangle \langle v_{s,\ell} | \chi \rangle + \frac{2}{\pi} \int_0^\infty \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle dk' \tag{58}$$

where $\langle \Phi | \chi \rangle$ is the standard Dirac notation

$$\langle \Phi | \chi \rangle = \int_0^\infty \Phi^{(*)}(r) \chi(r) dr. \tag{59}$$

As in the previous section, we shall assume that the Jost function $f_\ell(-k)$ has a double zero at $k = k_m$ in the fourth quadrant of the complex k' -plane, all other zeroes of $f_\ell(-k')$ in that quadrant being simple. Then, the scattering function $\psi_\ell^{(+)}(k', r)$ as function of k' -complex, has one double resonance pole at $k' = k_m$ and simple resonance poles at $k = k_n, n = 1, 2, \dots, m - 1, m + 1 \dots$, all in the fourth quadrant of the complex k' -plane. The function $\psi^{(+)*}(k', r)$ is regular and has no poles in the lower half of the k' -plane.

To make explicit the contribution of the resonant states to the expansion in eigenfunctions, the integration contour in the second term on the right-hand side of (58) is deformed as shown in Fig. 1. When the deformed contour C crosses over

resonant poles, the theorem of the residue gives

$$\begin{aligned} \langle \Phi | \chi \rangle &= \sum_{\substack{s \text{ bound} \\ \text{states}}} \langle \Phi | v_{s,\ell} \rangle \langle v_{s,\ell} | \chi \rangle \\ &+ \sum_{\substack{\text{all resonance} \\ \text{poles}}} 2\pi i \text{Res} \left[\frac{2}{\pi} \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle \right] \\ &+ \frac{2}{\pi} \int_C \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle dk'. \end{aligned} \tag{60}$$

The residues may be readily computed from Eqs. (11) and (60).

When $f_\ell(-k')$ has a simple zero at $k' = k_n$,

$$\begin{aligned} &2\pi i \text{Res} \left[\frac{2}{\pi} \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle \right]_{k'=k_n} \\ &= 4i \text{Res} \left[\frac{\langle \Phi | \phi_\ell(k') \rangle \langle \phi_\ell(k') | \chi \rangle k'^{2(\ell+1)}}{(k' - k_n) \left(\frac{df_\ell(-k')}{dk'} \right)_{k_n} f_\ell(k')} \right]_{k'=k_n} \\ &= \frac{1}{\frac{f_\ell(k_n)}{4ik_n^{2(\ell+1)}} \left(\frac{df_\ell(-k')}{dk'} \right)_{k_n}} [\langle \Phi | \phi_\ell(k') \rangle]_{k'=k_n} [\langle \phi_\ell(k') | \chi \rangle]_{k'=k_n}, \end{aligned} \tag{61}$$

where

$$[\langle \Phi | \phi_\ell(k') \rangle]_{k'=k_n} = \lim_{k' \rightarrow k_n} \int_0^\infty \Phi^*(r) \phi_\ell(k', r) dr, \tag{62}$$

and, since $\phi_\ell(k', r)$ is real for k' real,

$$[\langle \phi_\ell(k') | \chi \rangle]_{k'=k_n} = \lim_{k' \rightarrow k_n} \int_0^\infty \phi_\ell(k', r) \chi(r) dr. \tag{63}$$

Now, since $\phi_\ell(k_n, r)$ is an outgoing wave which oscillates between envelopes that grow exponentially at infinity and $\Phi(r)$ and $\chi(r)$ are very well behaved functions of r that decrease at infinity faster than any exponential, the integrals of the products $\Phi^*(r)\phi_\ell(k_n, r)$ and $\phi_\ell(k_n, r)\chi(r)$ exist, and we may take the limit indicated in the right-hand side of Eqs. (62) and (63) under the integration sign. The coefficient $4ik_n^{2(\ell+1)}[f_\ell(k_n)(df_\ell(-k')/dk')_{k_n}]^{-1}$ is the inverse of the normalization constant $N_{n\ell}^2$ defined in (29).

Therefore,

$$\begin{aligned} &2\pi i \text{Res} \left[\frac{2}{\pi} \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle \right]_{k'=k_n} \\ &= \langle \Phi | u_{u\ell}(k_n) \rangle \langle u_{n\ell}(k_n) | \chi \rangle \end{aligned} \tag{64}$$

where the notation means,

$$\langle \Phi | u_{n\ell}(k_n) \rangle = \int_0^\infty \Phi^*(r) u_{n\ell}(k_n, r) dr \tag{65}$$

and

$$(u_{n\ell}(k_n) | \chi) = \int_0^\infty u_{n\ell}(k_n, r) \chi(r) dr, \tag{66}$$

the function $u_{n\ell}(k_n, r)$ is the normalized Gamow eigenfunction defined in (17), (18), and (29).

When $f_\ell(-k')$ has a double zero at $k' = k_m$, $\psi_\ell^{(+)}(k', r)$ has a double pole at $k' = k_m$ and the residue of the term $2/\pi \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle$ at $k' = k_m$ is given by

$$\begin{aligned} & 2\pi i \text{Res} \left[\frac{2}{\pi} \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle \right]_{k'=k_m} \\ &= 4i \text{Res} \left[\frac{\langle \Phi | \phi_\ell(k') \rangle \langle \phi_\ell(k') | \chi \rangle k'^{2(\ell+1)}}{(k' - k_m)^2 g_{\ell m}(k') f_\ell(k')} \right]_{k'=k_m} \\ &= 4i \left[\frac{d}{dk'} \left(\frac{\langle \Phi | \phi_\ell(k') \rangle \langle \phi_\ell(k') | \chi \rangle k'^{2(\ell+1)}}{g_{\ell m}(k') f_\ell(k')} \right) \right]_{k'=k_m}, \end{aligned} \tag{67}$$

the function $g_{\ell m}(k')$ is given in (30) and (31).

After computing the derivative indicated in (67) and rearranging some terms, we obtain

$$\begin{aligned} & 2\pi i \text{Res} \left[\frac{2}{\pi} \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle \right]_{k'=k_m} \\ &= \frac{1}{\mathcal{N}_{m\ell}^2} [\langle \Phi | \hat{\phi}_\ell(k_m) \rangle \langle \phi_\ell(k_m) | \chi \rangle \\ & \quad + \langle \Phi | \phi_\ell(k_m) \rangle \langle \hat{\phi}_\ell(k_m) | \chi \rangle], \end{aligned} \tag{68}$$

the nonnormalized generalized Gamow–Jordan eigenfunction $\hat{\phi}_\ell(k_m, r)$ and the normalization constant $\mathcal{N}_{m\ell}^2$ are given in Eqs. (37) and (39) respectively. As in the computation of the residue at a simple pole, when $\Phi(r)$ and $\chi(r)$ are very well behaved functions of r , the limit $k' \rightarrow k_m$ can be taken under the integration sign.

Hence,

$$\begin{aligned} & 2\pi i \text{Res} \left[\frac{2}{\pi} \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle \right]_{k'=k_m} \\ &= \langle \Phi | \hat{u}_{m\ell}(k_m) \rangle (u_{m\ell}(k_m) | \chi) \\ & \quad + \langle \Phi | u_{m\ell}(k_m) \rangle (\hat{u}_{m\ell}(k_m) | \chi), \end{aligned} \tag{69}$$

where, the notation means

$$\langle \Phi | \hat{u}_{m\ell}(k_m) \rangle = \int_0^\infty \Phi^*(r) \hat{u}_{m\ell}(k_m, r) dr \tag{70}$$

and

$$(\hat{u}_{m\ell}(k_m) | \chi \rangle = \int_0^\infty \hat{u}_{m,\ell}(k_m, r) \chi(r) dr, \tag{71}$$

$\hat{u}_{m\ell}(k_m, r)$ is defined in (41).

Finally, substitution of the expressions (64) and (69) in (60) gives the following expansion:

$$\begin{aligned} \langle \Phi | \chi \rangle &= \sum_{\substack{s \text{ bound} \\ \text{states}}} \langle \Phi | v_{s\ell} \rangle \langle v_{s\ell} | \chi \rangle \\ &+ \sum_{\substack{n \neq m \\ \text{resonances}}} \langle \Phi | u_{n\ell} \rangle \langle u_{n\ell} | \chi \rangle \\ &+ \langle \Phi | \hat{u}_{m\ell}(k_m) \rangle \langle u_{m\ell}(k_m) | \chi \rangle \\ &+ \langle \Phi | \hat{u}_{m\ell}(k_m) \rangle \langle \hat{u}_{m\ell}(k_m) | \chi \rangle \\ &+ \frac{2}{\pi} \int_c \langle \Phi | \psi_\ell^{(+)}(k') \rangle \langle \psi_\ell^{(+)}(k') | \chi \rangle dk'. \end{aligned} \tag{72}$$

This expression shows that, when the Jost function has many simple zeroes and one double zero in the fourth quadrant of the complex k -plane, the Gamow eigenfunctions $u_{n\ell}(k_m, r)$ associated to simple zeroes of the Jost function and the chain $\{u_{m\ell}(k_m, r), \hat{u}_{m\ell}(k_m, r)\}$ of Gamow–Jordan eigenfunctions associated to the double pole of the Jost function are basis elements of an expansion in generalized bound and resonant state eigenfunctions plus a continuum of scattering functions of complex wave values k' .

Omitting the arbitrary function $\Phi(r)$ in (72), we obtain the complex basis expansion of an arbitrary square integrable and well-behaved function $\chi(r)$

$$\begin{aligned} \chi(r) &= \sum_{\substack{s \text{ bound} \\ \text{states}}} v_{s\ell}(r) \langle v_{s\ell} | \chi \rangle + \sum_{n \neq m} u_{n\ell}(k_n, r) \langle u_{n\ell} | \chi \rangle \\ &+ \hat{u}_{m\ell}(k_m, r) \langle u_{m\ell} | \chi \rangle + u_{m\ell}(k_m, r) \langle \hat{u}_{m\ell} | \chi \rangle \\ &+ \frac{2}{\pi} \int_c \psi_\ell^{(+)}(k', r) \langle \psi_\ell^{(+)}(k') | \chi \rangle, dk'. \end{aligned} \tag{73}$$

In this expression $u_{n\ell}(k_n, r)$ are the Gamow eigenfunctions representing decaying states associated to simple resonance poles of the scattering matrix $S(k)$ and the Green's function $G^{(+)}(k; r, r')$ and $\{u_{m\ell}(k_m, r), \hat{u}_{m\ell}(k_m, r)\}$ is the Jordan chain of length two of generalized Gamow–Jordan eigenfunctions associated to the double pole of the scattering matrix $S(k)$ and the Green's function $G^{(+)}(k; r, r')$ at $k = k_m$.

The last term on the right-hand side of (73) is the background integral defined along the integration contour shown in Fig. 1.

9. JORDAN BLOCKS IN THE COMPLEX ENERGY REPRESENTATION

Once it has been established that the Gamow eigenfunctions $u_{n\ell}(k_n, r)$ and the Jordan chain $\{u_{m\ell}(k_m, r), \hat{u}_{m\ell}(k_m, r)\}$ of generalized Gamow–Jordan eigenfunctions are elements of the basis set of eigenfunctions in the expansions (72) and (73), we may represent any operator $f(H_r^{(\ell)})$, which is a regular function of the Hamiltonian $H_r^{(\ell)}$, in terms of its matrix elements in this basis.

Let us start by deriving an expression for the action of $f(H_r^{(\ell)})$ on the generalized Gamow–Jordan eigenfunction $\hat{u}_{m\ell}(k_m, r)$. With this purpose in mind, let us write the eigenvalue equation satisfied by $u_{m\ell}(k_m, r)$ as

$$H_r^{(\ell)} u_{m\ell}(k_m, r) = \mathcal{E}_m u_{m\ell}(k_m, r), \tag{74}$$

where,

$$H_r^{(\ell)} = \frac{\hbar^2}{2\mu} \left[\frac{d^2}{dr^2} - v(r) - \frac{\ell(\ell + 1)}{r^2} \right] \tag{75}$$

$v(r)$ is a well-behaved short-ranged potential which satisfies the conditions stated in Section 1. Now, let us consider a holomorphic function $f(\mathcal{E})$ of the complex variable \mathcal{E} , such that,

$$f(\mathcal{E}) = \sum_{j=0}^{\infty} a_j \mathcal{E}^j, \tag{76}$$

the coefficients a_j are independent of \mathcal{E} .

Then, from (74) and (76),

$$f(H_r^{(\ell)}) u_{m\ell}(k_m, r) = f(\mathcal{E}_m) u_{m\ell}(k_m, r). \tag{77}$$

Taking derivatives with respect to the eigenvalue \mathcal{E}_m on both sides of (77), we obtain

$$f(H_r^{(\ell)}) \frac{\partial u_{m\ell}(k_m, r)}{\partial \mathcal{E}_m} = f(\mathcal{E}_m) \frac{\partial u_{m\ell}(k_m, r)}{\partial \mathcal{E}_m} + \frac{\partial f(\mathcal{E}_m)}{\partial \mathcal{E}_m} u_{m\ell}(k_m, r). \tag{78}$$

From this equation and the definition, Eqs. (37)–(41), of $\hat{u}_{m\ell}(k_m, r)$, it follows immediately that

$$f(H_r^{(\ell)}) \hat{u}_{m\ell}(k_m, r) = f(\mathcal{E}_m) \hat{u}_{m\ell}(k_m, r) + \frac{\partial f(\mathcal{E})}{\partial \mathcal{E}_m} u_{m\ell}(k_m, r). \tag{79}$$

Notice that a necessary and sufficient condition for the existence of $\partial u_{m\ell}(k_m, r) / \partial \mathcal{E}_m$ is the vanishing of $(df(-k)/dk)_{k_m}$.

The rule stated in Eq. (79) permits us to calculate the action of $f(H_r^{(\ell)})$ on the generalized Gamow–Jordan vectors occurring in the complex basis expansions (72) and (73).

Now, we can write the operator $f(H_r^{(\ell)})$ in terms of its matrix elements in the complex energy basis. This may be done by acting with $f(H_r^{(\ell)})$ on the left on both sides of Eq. (73),

$$\begin{aligned}
 f(H_r^{(\ell)})\chi(r) &= \sum_s f(\mathcal{E}_s)v_{s\ell}(r)\langle v_{s\ell}|\chi\rangle \\
 &+ \sum_{n \neq m} f(\mathcal{E}_n)u_{n\ell}(k_n, r)\langle u_{n\ell}|\chi\rangle \\
 &+ \left(f(\mathcal{E}_m)\hat{u}_{m\ell}(k_m, r) + \frac{\partial f(\mathcal{E}_m)}{\partial \mathcal{E}_m}u_{m\ell}(k_m, r) \right) \langle u_{m\ell}|\chi\rangle \\
 &+ f(\mathcal{E}_m)u_{m\ell}(k_m, r)\langle \hat{u}_{m\ell}|\chi\rangle \\
 &+ \frac{2}{\pi} \int_c f(\mathcal{E}')\psi_\ell^{(+)}(k', r)\langle \psi_\ell^{(+)}(k')|\chi\rangle, dk'. \tag{80}
 \end{aligned}$$

Multiplying both sides of (80) by $\Phi^*(r)$ and integrating over r , we get

$$\begin{aligned}
 \langle \Phi|f(H_r^{(\ell)})|\chi\rangle &= \sum_s \langle \Phi|v_{s\ell}\rangle f(\mathcal{E}_s)\langle v_{s\ell}|\chi\rangle \\
 &+ \sum_{n \neq m} \langle \Phi|u_{n\ell}\rangle f(\mathcal{E}_n)\langle u_{n\ell}|\chi\rangle + \langle \Phi|\hat{u}_{m\ell}\rangle f(\mathcal{E}_m)\langle u_{m\ell}|\chi\rangle \\
 &+ \langle \Phi|u_{m\ell}\rangle \left(f(\mathcal{E}_m)\langle \hat{u}_{m\ell}|\chi\rangle + \frac{\partial f(\mathcal{E}_m)}{\partial \mathcal{E}_m}\langle u_{m\ell}|\chi\rangle \right) \\
 &+ \frac{2}{\pi} \int_c \langle \Phi|\psi_\ell^{(+)}(k')\rangle f(\mathcal{E}')\langle \psi_\ell^{(+)}(k')|\chi\rangle, dk'. \tag{81}
 \end{aligned}$$

To simplify the notation, suppose that the system has no bound states only resonances and that the first two resonances are degenerate. Rearranging Eq. (81) in matrix form, we get

$$\begin{aligned}
 \langle \Phi|f(H_r^{(\ell)})|\chi\rangle &= (\langle \Phi|u_{1\ell}\rangle, \langle \Phi|\hat{u}_{1\ell}\rangle, \langle \Phi|u_{3\ell}\rangle, \dots) \\
 &\times \begin{pmatrix} f(\mathcal{E}_1) & \frac{\partial f(\mathcal{E}_1)}{\partial \mathcal{E}_1} & 0 & 0 & 0 & 0 \dots \\ 0 & f(\mathcal{E}_1) & 0 & 0 & 0 & 0 \dots \\ 0 & 0 & f(\mathcal{E}_3) & 0 & 0 & 0 \dots \\ 0 & 0 & 0 & f(\mathcal{E}_4) & 0 & 0 \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} \langle \hat{u}_{1\ell}|\chi\rangle \\ \langle u_{1\ell}|\chi\rangle \\ \langle u_{3\ell}|\chi\rangle \\ \vdots \end{pmatrix} \\
 &+ \frac{2}{\pi} \int_c \langle \Phi|\psi_\ell^{(+)}(k')\rangle f(\mathcal{E}')\langle \psi_\ell^{(+)}(k')|\chi\rangle dk'. \tag{82}
 \end{aligned}$$

In this matrix representation of $f(H_r^{(\ell)})$,⁴ the upper left 2×2 submatrix is a Jordan block of rank 2 associated to the chain of Gamow–Jordan generalized eigenfunctions $\{\hat{u}_{1\ell}(k_1, r), u_{1\ell}(k_1, r)\}$ belonging to the double zero of the Jost function $f_\ell(-k)$ (double pole of the scattering matrix and the Green’s function). Except for this 2×2 block, this matrix is diagonal with the eigenvalues $f(\mathcal{E}_n)$ in the diagonal entries. Simple zeroes of the Jost function correspond to simple (nonrepeated) eigenvalues of $f(H_r^{(\ell)})$ while the double zero of $f_\ell(-k)$ correspond to the twice repeated (degenerate) eigenvalue $f(\mathcal{E}_1)$ occurring in the Jordan block. The off-diagonal non-vanishing element in this block is $\partial f(\mathcal{E}_1)/\partial \mathcal{E}_1$.

The difference in physical dimensions of the off-diagonal and the diagonal entries in the 2×2 Jordan block is compensated by the difference in normalization of the Gamow–Jordan chain $\{\hat{u}_{1\ell}(k_1, r), u_{1\ell}(k_1, r)\}$ and the Gamow eigenfunctions $u_{n\ell}(k_n, r)(n = 3, 4, \dots)$ which are normalized according to (40 and 41) and (17) and (29) respectively.

It will be instructive to consider some simple examples.

We first choose $f(H_r^{(\ell)}) = H_r^{(\ell)}$. Then, from (82) we obtain

$$\begin{aligned} \langle \Phi | (H_r^{(\ell)}) | \chi \rangle &= (\langle \Phi | u_{1\ell} \rangle, \langle \Phi | \hat{u}_{1\ell} \rangle, \langle \Phi | u_{3\ell} \rangle, \dots) \\ &\times \begin{pmatrix} \mathcal{E}_1 & 1 & 0 & 0 & 0 & 0 & \dots \\ 0 & \mathcal{E}_1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & \mathcal{E}_3 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & \mathcal{E}_4 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \langle \hat{u}_{1\ell} | \chi \rangle \\ \langle u_{1\ell} | \chi \rangle \\ \langle u_{3\ell} | \chi \rangle \\ \vdots \end{pmatrix} \\ &+ \frac{2}{\pi} \int_c \langle \Phi | \psi_\ell^{(+)}(k') \rangle \mathcal{E}' \langle \psi_\ell^{(+)}(k') | \chi \rangle, dk'. \end{aligned} \tag{83}$$

From this example, it is evident that in a degeneracy of two resonances in the absence of symmetry, the degenerate complex eigenvalue \mathcal{E}_1 occurs twice in the spectral representation of the radial Hamiltonian $H_r^{(\ell)}$ given in (83), while there is only one Gamow eigenvector or normal mode, $u_{1\ell}(k_1, r)$, associated to the degeneracy. This is so, because the Gamow–Jordan generalized eigenfunction or abnormal mode, $\hat{u}_{1\ell}(k_1, r)$, is not an eigenfunction of the radial Hamiltonian $H_r^{(\ell)}$. This is a generic property of this kind of degeneracy which may be stated in slightly more formal terms as follows. In a degeneracy of resonances in the absence of symmetry, the algebraic multiplicity is always larger than the geometric multiplicity. Here, we mean by algebraic multiplicity of a degeneracy, μ_a , the number of times the degenerate complex eigenvalue is repeated, and, by geometric multiplicity of the

⁴From the way it was derived, it is evident that the matrix in Eq. (82) represents the action of $f(H_r^{(\ell)})$ as an operator on the space of continuous antilinear functionals on the Schwarz space of very well behaved test functions.

degeneracy, μ_g , the dimensionality of the subspace spanned by the eigenvectors associated to the degenerate eigenvalue (Lancaster and Tismenetsky, 1985).

Then,

$$\mu_a > \mu_g. \tag{84}$$

Let us consider now the complex energy representation of the resolvent operator. In this case $f(H_r^{(\ell)}) = 1/(E^+ - H_r^{(\ell)})$, then, from (82), we obtain

$$\begin{aligned} \langle \Phi | \frac{1}{E - H_r^{(\ell)}} | \chi \rangle &= (\langle \Phi | u_{1\ell} \rangle, \langle \Phi | \hat{u}_{1\ell} \rangle, \langle \Phi | u_{3\ell} \rangle, \dots) \\ &\times \begin{pmatrix} \frac{1}{E - \mathcal{E}_1} & \frac{1}{(E - \mathcal{E}_1)^2} & 0 & 0 & 0 & 0 & \dots \\ 0 & \frac{1}{E - \mathcal{E}_1} & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & \frac{1}{E - \mathcal{E}_3} & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & \frac{1}{E - \mathcal{E}_4} & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} \langle \hat{u}_{1\ell} | \chi \rangle \\ \langle u_{1\ell} | \chi \rangle \\ \langle u_{3\ell} | \chi \rangle \\ \vdots \end{pmatrix} \\ &+ \frac{2}{\pi} \int_c \langle \Phi | \psi_\ell^{(+)}(k') \rangle \frac{1}{(E - \mathcal{E}') } \langle \psi_\ell^{(+)}(k') | \chi \rangle, dk'. \end{aligned} \tag{85}$$

It may easily be verified that, when we delete the arbitrary functions $\Phi(r)$ and $\chi(r)$ in this expression, the resulting expansion for $\langle r | \frac{1}{E - H_r^{(\ell)}} | r' \rangle$ is equal to the expansion in resonance eigenfunctions of the complete Green’s function given in Eq. (43) which was derived in Section 5 directly from the spectral representation of $G_\ell^{(+)}(k; r, r')$. The occurrence of the double pole in $G_\ell^{(+)}(k; r, r')$, as function of the complex energy, is thus associated to the occurrence of a Jordan block of rank 2 in the complex basis representation of the resolvent operator and a Jordan chain of Gamow–Jordan generalized eigenfunctions $\{\hat{u}_{1\ell}(k_1, r), u_{1\ell}(k_1, r)\}$.

Finally, let us consider the time evolution operator $\exp(-iHt)$. For each fixed value of the angular momentum, it will be enough to consider the operator $f(H_r^{(\ell)}) = \exp(-iH_r^{(\ell)}t)$. In this case, from Eq. (82)

$$\begin{aligned} \langle \Phi | \exp(-iH_r^{(\ell)}t) | \chi \rangle &= (\langle \Phi | u_{1\ell} \rangle, \langle \Phi | \hat{u}_{1\ell} \rangle, \langle \Phi | u_{3\ell} \rangle, \dots) \\ &\times \begin{pmatrix} \exp(-i\mathcal{E}_1t) & -it \exp(-i\mathcal{E}_1t) & 0 & 0 & 0 & \dots \\ 0 & \exp(-i\mathcal{E}_1t) & 0 & 0 & 0 & \dots \\ 0 & 0 & \exp(-i\mathcal{E}_3t) & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} \langle \hat{u}_{1\ell} | \chi \rangle \\ \langle u_{1\ell} | \chi \rangle \\ \langle u_{3\ell} | \chi \rangle \\ \vdots \end{pmatrix} \\ &+ \frac{2}{\pi} \int_c \langle \Phi | \psi_\ell^{(+)}(k') \rangle \exp(-i\mathcal{E}'t) \langle \psi_\ell^{(+)}(k') | \chi \rangle, dk'. \end{aligned} \tag{86}$$

As in the previous examples, the time evolution operator is nondiagonal in the complex energy basis representation. The time evolution of the Jordan chain

of Gamow–Jordan generalized eigenfunctions $\{\hat{u}_{1\ell}(k_1, r), u_{1\ell}(k_1, r)\}$ is given by a Jordan block of 2×2 with an exponential time dependence in the diagonal entries and a first order polynomial times an exponential in the off-diagonal entry. Hence, the time evolution of the Gamow–Jordan generalized eigenfunction or abnormal mode is a superposition of the abnormal mode $\hat{u}_{1\ell}(k_1, r)$ evolving exponentially in time plus the normal mode $u_{1\ell}(k_1, r)$ evolving according to the product of a first-order polynomial times an exponential time evolution factor. The time evolution of the normal mode $u_{1\ell}(k_1, r)$ in the Gamow–Jordan chain $\{\hat{u}_{1\ell}(k_1, r), u_{1\ell}(k_1, r)\}$, as well as the time evolution of all other normal modes $u_{n\ell}(k_n, r)$ associated to the simple zeroes of the Jost function (simple poles of the scattering matrix), is purely exponential.

10. SUMMARY AND CONCLUSIONS

In a one-channel scattering problem, degeneracy of resonances, that is, the exact coincidence of two (or more) simple resonance poles of the scattering matrix and the complete Green's function, arises from the exact coincidence of two (or more) simple resonance zeroes of the Jost function which merge into one second (or higher) rank resonance zero of the same function lying in the fourth quadrant of the complex k -plane.

We found that, associated to a double resonance zero of the Jost function, there is a Jordan chain of length two of generalized Gamow–Jordan eigenfunctions $\{\hat{u}_{m\ell}(k_m, r), u_{m\ell}(k_m, r)\}$ belonging to the same degenerate complex energy eigenvalue \mathcal{E}_m . In consequence, the corresponding second-rank pole occurring in the scattering matrix, $S_\ell(k)$, the Green's function, $G_\ell^{(+)}(k; r, r')$ and the scattering wave function $\psi_\ell^{(+)}(k, r)$ is also associated to this Jordan chain of Gamow–Jordan generalized resonance eigenfunctions. Explicit expressions for the normalized Gamow and Gamow–Jordan generalized eigenfunctions in this chain, written in terms of the outgoing wave Jost solution, the Jost function and its derivatives evaluated at the double zero, are obtained from the computation of the residue of the Green's function at the double pole.

We also showed that the Jordan chain of generalized eigenfunctions are elements of the complex biorthonormal basis formed by the real (bound states) and complex (resonance states) energy eigenfunctions which can be completed by means of a continuum of scattering wave functions of complex wave number. With the help of this result, we derived expansion theorems (spectral representations) for operators $f(H_r^{(\ell)})$ which are regular functions of the radial Hamiltonian $H_r^{(\ell)}$. In this basis, the operator $f(H_r^{(\ell)})$ is represented by a complex matrix which is diagonal except for one Jordan block of rank 2 associated to the double zero of the Jost function and the corresponding chain of generalized eigenvectors. The diagonal entries in this matrix are the eigenvalues $f(\mathcal{E}_n)$, simple zeroes of the Jost function correspond to nondegenerate eigenvalues of $f(H_r^{(\ell)})$ while the double zero of the

Jost function corresponds to the twice repeated (degenerate) eigenvalue $f(\mathcal{E}_m)$ in the diagonal entries of the Jordan block. The off-diagonal, non-vanishing element in this block is $\partial f(\mathcal{E}_m)/\partial \mathcal{E}_n$. In particular, the occurrence of a double pole in the Green's function, as function of the complex energy, is thus associated to the occurrence of a Jordan block of rank 2 in the complex basis representation of the resolvent operator and the corresponding Jordan chain of Gamow–Jordan generalized eigenfunctions.

Finally, let us stress the fact that in the Gamow–Jordan chain of generalized eigenfunctions $\{\hat{u}_{m\ell}(k_m, r), u_{m\ell}(k_m, r)\}$ associated to the double zero of the Jost function, there is only one eigenvector, namely the Gamow eigenfunction or normal mode $u_{m\ell}(k_m, r)$. The Gamow–Jordan generalized eigenfunction or abnormal mode $\hat{u}_{m\ell}(k_m, r)$ is not an eigenfunction of the radial Hamiltonian. Hence, the dimensionality of the subspace of eigenfunctions associated to the degeneracy of two resonances or geometric multiplicity, μ_g , of the degeneracy is one. But, the number of times the degenerate complex energy eigenvalue is repeated in the spectral representation of $H_r^{(\ell)}$ or algebraic multiplicity of the degeneracy, μ_a , is two. Therefore, the algebraic multiplicity is larger than the geometric multiplicity of a degeneracy of resonances. This is a generic property of a degeneracy of resonances in the absence of symmetry.

ACKNOWLEDGMENTS

We thank Prof A. Bohm (Univ. of Texas at Austin) and Prof P. von Brentano (Univ. zu Köln) for many inspiring discussions on this exciting problem. This work was supported by CONACyT México under contract number 40162-F and by DGAPA-UNAM contract No. PAPIIT:IN116202.

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