Resonant state expansion of the resolvent

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An analytic method of generating resonant state expansions from the standard completeness relation of nonrelativistic quantum mechanics is described and shown to reproduce the generalized completeness relations, earlier derived, involving resonant states. The method is then applied to the expansion of the resolvent (the complete Green's function), the symmetry properties of which *seem* to be destroyed if a conventional application of the completeness relations is made. These forms of expansions have a continuum term which contains symmetry-restoring contributions and can therefore never vanish identically, nor can it be neglected. The symmetry-conserving form of the expansion has a set of discrete terms which are identical in form to those of the Mittag-Leffler series for the resolvent. In addition, it contains a continuum contribution which in some cases vanishes identically, but in general does not. We illustrate these findings with numerical applications in which the potential (a square well) is chosen so as to permit analytic evaluation of practically all functions and quantities involved.

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I. INTRODUCTION

Until about two decades ago the concept of a resonant (or *Gamow*) state, founded in Gamow's original idea [1] concerning the quantal description of a radioactive state, was too vague and exotic to be incorporated as a truly physical element in the theory of nuclear or atomic systems. Gamow's idea was taken up by Siegert [2] in 1939 and then, in the early 1960s, used by Rosenfeld and Humblet [3] in a comprehensive theory of nuclear reactions. It was soon found, however, that the analogy between bound and radioactive states was much closer than one had until then believed, and theories of Gamow wave functions were formulated with prescriptions for how to normalize such functions [4, 5] and how to form inner products [6, 7] from them. This enabled the use of such states not only in reaction calculations but also as *structure* elements, albeit structures of a more or less temporary character. The new feature was the establishment of completeness relations [6] involving Gamow states. Completeness directly provides the possibility to expand wave functions as well as scattering and reaction amplitudes in terms of resonant states. The Rosenfeld-Humblet theory [3], on the other hand, is based on the Mittag-Leffler expansion of the scattering amplitude, involving a theorem on meromorphic functions which somewhat obscures the role of the resonant wave functions and the analogy with ordinary perturbation theory. A certain amount of rivalry has existed between those who prefer the Mittag-Leffler formulation and those who feel more at home with eigenfunction expansions. One of the aims of this paper is to show that the two forms of approach can be reconciled.

It must be admitted that in the early days of resonant state expansions we had a tendency to underestimate the importance of a characteristic property of the completeness relations: they all contain an integral over a set of continuum states. Tacitly and without proof one often assumed that if one chooses this set suitably and includes the physically important resonances in the expansion, then the continuum contribution to physical quantities would be negligibly small. In other words, there would be no residual effects from the continuum if all resonances could be taken into account. To a large extent this expectation could feed on the results of the Mittag-Leffler formalism, which leads to a sum over discrete resonant state terms to which is added a term in the form of an entire function, the value of which could be manipulated by modifying the form of the discrete terms. It must also be remembered that actually calculating the continuum contribution in a nontrivial case involves a great deal of numerical effort. Therefore few attempts to test the assumption of a negligible continuum contribution have been made up to now. The so-called continuum shell model [8] tackles the problem differently and gives little guidance for the problem of continuum contributions to resonant state expansions. The present paper reports on the first phase of a study which is aimed at clarifying the role of the resonant states in the continuum problem.

Of particular interest is the resonant state expansion of the resolvent or complete Green's function, which plays a central role in perturbation theory, especially the random phase approximation (RPA). In this field recent work [9–13] aiming at introducing Gamow state expansions into the continuum RPA has proved very successful. However, although the resonant state expansions derived in accordance with Ref. [6] proved to be conceptually very fruitful, their numerical accuracy, although acceptable in the vicinity of the resonances, was elsewhere less satisfactory than that of the Mittag-Leffler expansions. Experience gained in Ref. [14] pointed in the same direction, viz. that in order to get a good approximation for the resolvent its usual form must be modified so as to eliminate the spurious poles of this form. This was pointed out in a perturbation-theoretical analysis by Romo [15]. We have found, in addition, that if one uses the completeness relations to expand the resolvent one may destroy the symmetry properties of this operator. This can be avoided by using a method outlined in Ref. [14] and described briefly in Sec. II, where a summary of the most often used completeness relations is presented and commented. In Sec. III this method is applied to the resolvent yielding a resonant state expansion which has discrete terms similar to those of the Mittag-Leffler theory but also contains a continuum integral. The validity of the approximation of keeping only the discrete terms in various forms of the resolvent expansion is illustrated in Sec. III B.

II. REVIEW OF THE THEORETICAL BACKGROUND

In Ref. [6] use was made of the fact that the continuum radial amplitudes, for given orbital angular momentum $\hbar\ell$, as defined by Newton [16]

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

have poles $k = k_n$ and $k = \tilde{k}_n \equiv -k_n^*$ at the zeros of the Jost function [17] $f_\ell(-k)$. For a large class of potentials including the finite-range ones the functions $\varphi_\ell(k,r)$ are entire functions of the wave number k and satisfy the boundary condition

$$\lim_{r\to 0} \frac{(2\ell+1)!!\varphi_\ell(k,r)}{r^{\ell+1}} = 1.$$

A direct consequence of this condition is that

$$\lim_{r\to 0} \frac{\dot{\varphi}_\ell(k,r)}{r^{\ell+1}} = 0,$$

where, as in the following, the dot over the symbol indicates derivation with respect to k. Equivalently,

$$\lim_{r\to 0} \frac{\dot{\varphi}_\ell(k,r)}{\varphi_\ell(k,r)} = 0. \tag{2}$$

The completeness relation for the bound states u_b and the (real momentum) scattering states (1) may be written

$$\delta(r-r') = \sum_b u_b(r)u_b(r') + \frac{2}{\pi}\int_0^\infty dk\, \psi_\ell(k,r)\psi_\ell^*(k^*,r'). \tag{3}$$

Here we have used $u_n(r) = \varphi_\ell(k_n,r)/N$ with the normalization constant from

$$N^2 = \int_0^\infty dr\, \varphi_\ell(k_n,r)^2, \tag{4}$$

where the integral is to be defined by means of a suitable regularization procedure whenever $u_n(r)$ is a resonant or antibound wave function. This normalization is equivalent to that obtained by demanding $u_n(r)u_n(r')$ to be given by the residue of the resolvent (see below) at $k = k_n$.

The properties of $\varphi_\ell(k,r)$ imply

$$\tilde{u}_n(r) = \varphi_\ell(k_n^*,r)/N^* = u_n^*(r).$$

For real momenta, the complex conjugation of k in the second factor of the integrand of (3) is of course immaterial. However, Eq. (3) is written here in such a form that the integrand can be a meromorphic function of k in some region containing the real k axis, with poles at the zeros of $f_\ell(\pm k)$. The poles at $k = k_n^*$ and $k = -k_n$ have no counterpart in the resolvent $\mathcal{G}_\ell(k;r,r')$ (cf. Newton [16] and below, Sec. III). In the integrand of (3) the bound and antibound states also give rise to *two* poles, one in the upper and one in the lower half-plane.

Using definition (1), a relation [16, 6] (see also the Appendix) between the Jost functions at resonance, i.e., for $f_\ell(-k_n) = 0$, and the normalization integral for the bound and resonant states, viz.

$$f_\ell(k_n)\left.\frac{df_\ell(k)}{dk}\right|_{k=-k_n} = 4ik_n^{2\ell+2}N^2, \tag{5}$$

we find that the residue at $k = k_n$ of the integrand of (3) is

$$\mathrm{Res}_{k=k_n}[\psi_\ell(k,r)\psi_\ell^*(k^*,r')] = +\frac{1}{4}iu_n(r)\tilde{u}_n^*(r'). \tag{6a}$$

The symmetry relations [16] $f_\ell(k^*) = f_\ell^*(-k)$ from which follows $\dot{f}_\ell(k^*) = -\dot{f}_\ell^*(-k)$ give

$$\mathrm{Res}_{k=k_n^*}[\psi_\ell(k,r)\psi_\ell^*(k^*,r')] = -\frac{1}{4}i\tilde{u}_n(r)u_n^*(r'). \tag{6b}$$

We further get

$$\mathrm{Res}_{k=-k_n}[\psi_\ell(k,r)\psi_\ell^*(k^*,r')] = -\frac{1}{4}iu_n(r)\tilde{u}_n^*(r') \tag{6c}$$

and

$$\mathrm{Res}_{k=-k_n^*}[\psi_\ell(k,r)\psi_\ell^*(k^*,r')] = +\frac{1}{4}i\tilde{u}_n(r)u_n^*(r'). \tag{6d}$$

It is convenient to introduce an index convention for the discrete states, using the letter b to index the bound states ($\mathrm{Im}k_b > 0$), the letter a for the antibound (virtual) states ($\mathrm{Im}k_a < 0$), the letter d for the outgoing (decaying) resonances ($\mathrm{Re}k_d > 0$), and the letter c for the incoming (capturing) resonances ($\mathrm{Re}k_c < 0$). In this notation Eqs. (6a)–(6d) can be written using $u_c(r) = \tilde{u}_d(r)$ and $k_c = -k_d^*$:

$$\mathrm{Res}_{k=\pm k_n} = \pm\frac{i}{4}u_n(r)\tilde{u}_n^*(r'),$$

where n might be either of $a, b, c,$ or d since for the bound states we have $u_b(r) = \tilde{u}_b(r)$ and correspondingly for the antibound states.

We first make a note on the method which Newton [16] and Berggren [6] used to prove the completeness relation in terms of discrete and scattering states. They considered the integral

$$I^*(r) = \oint_{C'} k\,dk \int_0^\infty dr' h(r')\mathcal{G}_\ell(k;r,r'), \tag{7}$$

where the closed contour ($C' = C+S$) consists of a semicircle (S) in the upper half-plane and some path (C) from

$-\infty$ to ∞ through the origin, chosen so that C' includes the poles that one is interested in. If the continuum part of the resulting completeness relation is to be of familiar form, it is essential that the contour C is inversion symmetric, i.e., if k is on C then so is $-k$. (See Fig. 1 for contours relevant for this proof.) If we wish to separate the physical resonances from the wide ones whose energy has a negative real part (these resonances were not considered physical in [3] and will here be called *virtual resonances* to emphasize their similarity with the antibound states), we will draw all contours that go through $k = 0$ so that they form an angle $\leq \pi/4$ with the real k axis. (This angle was chosen in [6] because of the regularization procedure used there. If we use a different procedure, e.g., the complex rotation regularization [11], cf. also [18], the angle can be chosen $< \pi/2$.)

If we only consider functions $h(r')$ that are sufficiently well behaved asymptotically then we can use Cauchy's theorem to evaluate the integral $I^*(r)$ and express the resulting completeness relations as "resolutions of the identity" (more generally projection operators)

$$\mathbb{1} = \sum_{n=b} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_R |\psi(k)\rangle dk \langle\psi(k^*)| \qquad (8)$$

and

$$\mathbb{1} = \sum_{n=b,d} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_L |\psi(k)\rangle dk \langle\psi(k^*)|. \qquad (9)$$

Since the integrand in (8) [and in (3)] is meromorphic, we can also consider (9) to have been obtained from (8) by contour deformation using the residues (6a)–(6d). (The contours and pole structure for this method are seen in Fig. 2.) By deforming the contour into the Z contour we obtain the completeness relation suggested in [14]:

$$\mathbb{1} = \sum_{n=b,c,d} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_Z |\psi(k)\rangle dk \langle\psi(k^*)|. \qquad (10)$$

The purpose with introducing this contour is to separate from the L integral a resonance contribution which is complex conjugate to the discrete part in (9) so that the approximate expansion of a real function obtained by neglecting the integral will be real. This is not the case in

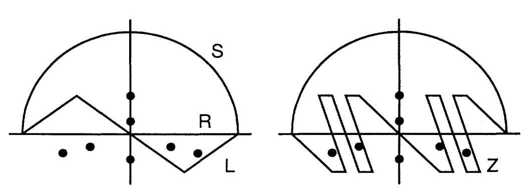

FIG. 1. Contours in the k plane for the integral (7) used in proofs of completeness relations. The dots mark the positions of the poles of $\mathcal{G}_\ell(k; r, r')$.

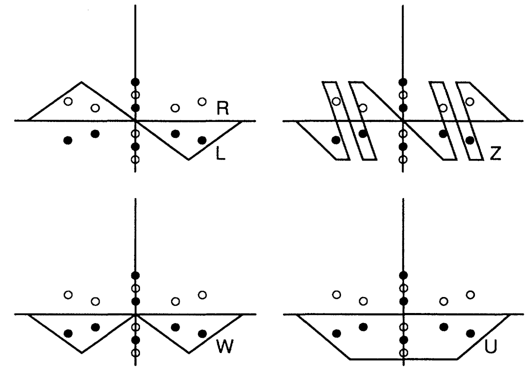

FIG. 2. Contours in the k plane that define the continuum in the resonant state expansions (8)–(11) and (19)–(21). The dots mark the positions of the poles of $\psi_\ell(k, r)$ and the circles mark the positions of the poles of $\psi_\ell^*(k^*, r)$.

the approximation[1] obtained by neglecting the integral in (9) which complicates the physical interpretation [6].

Using this method to the extreme by deforming the contour into the U contour (equivalent to an infinite semicircle in the lower half-plane in the case of a finite-range potential) we get [15]

$$\mathbb{1} = \tfrac{1}{2} \sum_{n=a,b,c,d} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_U |\psi(k)\rangle dk \langle\psi(k^*)|. \qquad (11)$$

where the sum corresponds term by term to the Mittag-Leffler expression for $\delta(r - r')$ as given by [19]. The work by Romo, in particular Ref. [20], shows that for functions which are strictly zero outside a radius smaller than the finite range of the potential (see further [20] for more specific conditions) the integral will vanish if the sum is taken over all discrete states. The completeness relations obtainable by invoking analyticity from that of Newton, Eq. (8), are thereby related with and sometimes equivalent to the Mittag-Leffler expansion. The U contour integral seems to be the only one that can be shown to vanish not only in special cases but for some class of functions. One can, on the other hand, give examples [21] of functions for which this integral has a finite value that *cannot* be expressed as a component with respect to any of the discrete states, nor can it be incorporated in the Mittag-Leffler expansion.

[1]Unfortunately it was not realized in Ref. [14] that the continuum contribution from the Z contour usually has a magnitude which is of the same order as the discrete part, so that neglecting it is in general a very poor approximation. Neglecting the continuum contribution from the L contour means, on the other hand, that a real quantity is approximated by a complex quantity whose real part we expect to be fairly accurate. The imaginary part (approximately the error) may be dominated by contributions from non-narrow resonances and thus difficult to estimate *a priori.*

Since the operator $\frac{1}{2}|u_n\rangle\langle\tilde{u}_n|$ is not idempotent and thus not a projection operator, we hesitate to call the discrete part of (11) a *completeness* relation. The factor $\frac{1}{2}$ is the result of extracting resolvent-pole contributions from the original continuum integral in Eq. (8) and combining them with the original discrete terms. The term "*overcompleteness relation*" suggested in Ref. [19] is neither fully adequate, as the linear dependence alluded to by this expression is only present in the region inside the finite range of the potential.[2] We will provisionally call relations of this kind which are not built from idempotent terms *reduced* completeness relations, referring to the reduction of the original projection operators by discrete contributions from the continuum integral.

It should be clear that neglecting the contribution from the continuum integral may result in approximate resonant state expansions with greatly differing accuracy, depending on which of the "completeness relations" presented above is taken as the point of departure. The validity, usefulness, and consequences of these "completeness relations" will be further studied in Ref. [21]. However, it has been found that if one tries to use these relations to derive resonant state expansions of the resolvent operator then one may run into difficulties with reproducing some of its basic properties such as pole positions and symmetries. How to obtain expansions of the resolvent which preserve its essential properties is the main subject of the present paper.

III. RESOLVENT

The *proof* of the completeness relation (3) given in Ref. [16] and modified in Ref. [6] for the inclusion of a finite number of resonant states is based on the properties of the resolvent (or *complete Green's function*):

$$\mathcal{G}_\ell(k;r,r') = \frac{(-1)^{\ell+1}k^\ell \varphi_\ell(k,r_<)f_\ell(-k,r_>)}{f_\ell(-k)} = \frac{(-1)^{\ell+1}}{k}\psi_\ell(k,r_<)f_\ell(-k,r_>), \tag{12}$$

where

$$r_> \equiv \max(r,r'), \qquad r_< \equiv \min(r,r').$$

The resolvent is a solution, regular at $r=0$, of

$$\left(-\frac{d^2}{dr^2} + V(r) + \frac{\ell(\ell+1)}{r^2} - k^2\right)\mathcal{G}_\ell(k;r,r') = -\delta(r-r'). \tag{13}$$

It has a well-defined asymptotic behavior in coordinate space [for Re(k) positive purely outgoing, or for Re(k) negative purely incoming, spherical waves]. Since both $f_\ell(-k,r)$ and $f_\ell(-k)$ are regular in the upper half of the k plane [16], the same is true for the resolvent except for poles due to the zeros k_n and $-k_n^*$ of $f_\ell(-k)$. Depending on the behavior of the potential $V(r)$ for large values of r the functions $f_\ell(-k,r)$, $f_\ell(-k)$ may be shown to be regular also, e.g., in a strip in the lower k plane along the real k axis and therefore $\mathcal{G}_\ell(k;r,r')$ at least meromorphic in the same domain. The poles outside the imaginary k axis occur only in the lower half of the k plane and represent *resonances* while those on the negative imaginary axis represent *antibound* states. All poles in the upper half-plane thus lie on the imaginary axis; they correspond to *bound* states. From the symmetry $f_\ell^*(-k^*,r) = (-1)^\ell f_\ell(k,r)$ (Ref. [16], Sec. III) we get

$$\mathcal{G}_\ell(-k^*;r,r') = \mathcal{G}_\ell^*(k;r,r'), \tag{14}$$

i.e., the resolvent is symmetric with respect to reflection in the imaginary k axis followed by complex conjugation. We should note that the substitution $k \to -k$ not only changes the asymptotic properties from outgoing waves to incoming waves and vice versa but also interchanges the analytic properties in the upper and lower half-planes. Thus $\mathcal{G}_\ell(-k;r,r')$ is a solution of Eq. (13) corresponding to a *different* boundary condition at the same energy. It is (for $k \neq 0$) linearly independent of $\mathcal{G}_\ell(k;r,r')$ and should therefore in principle be considered a different function. Its poles are the zeros of $f_\ell(k)$ and are found in the opposite half-plane compared to those of $\mathcal{G}_\ell(k;r,r')$.

The asymptotic behavior of the integrand of (3), however, is mixed in coordinate space. The analytic properties of the integrand as a function of k depend on the properties of the potential. We already know that the integrand has poles outside the real k axis and may have other singularities at some distance from the real k axis (see further [16]). For realistic potentials we may assume that apart from the poles it is analytic in a fairly broad strip containing the real axis. Therefore, once completeness is established and Eq. (3) is derived, that equation can be used as the starting point for deriving the various *forms* of completeness relations.

After proving the completeness relation (3) Newton [16] derives the expressions

$$\mathcal{G}_\ell^R(k;r,r') = \frac{2}{\pi}\int_0^\infty dq \frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k^2-q^2} + \Sigma_b = \frac{1}{\pi}\int_{-\infty}^\infty \frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k-q} + \Sigma_b, \tag{15}$$

where we use the abbreviation

$$\Sigma_b = \sum_b \frac{u_b(r)u_b(r')}{k^2+\gamma_b^2}. \tag{16}$$

Here the sum includes all the bound states with $k_b = i\gamma_b$. The integral is taken along the real axis (as specified by the superscript R) in the wave number (k or q) plane. We note that for k real the integral diverges due to the

[2] Obviously *completeness* is a property of a set of functions which implies that the set is (a) linearly independent and (b) saturated in the sense that if any function is adjoined to the set then the resulting set will be linearly dependent. This is why complete sets can be used as basis sets. Orthogonality helps to establish linear independence and to write down "completeness relations" but is not a necessary requirement.

pole at $q = k$ on the integration path, but for k complex the integral converges since the integrand is then bounded everywhere[3] and $O(q^{-2})$as $q \to \pm\infty$. Therefore the integral defines an analytic function of k outside the real axis. This axis is then a branch cut from $-\infty$ to $+\infty$. It is obvious that since the sum (16) has poles only on the imaginary k axis, and these poles are situated symmetrically with respect to the real k axis, Eq. (15) can only represent $\mathcal{G}_\ell(k;r,r')$ in the upper half-plane, and $\mathcal{G}_\ell(-k;r,r')$ in the lower half-plane. In other words, $\mathcal{G}_\ell^R(k;r,r')$ as defined by the eigenfunction expansion (15) cannot be considered as a one-valued function. The branch in the upper half-plane we may temporarily denote by $\mathcal{G}_\ell^{R+}(k;r,r')$, the branch in the lower half-plane by $\mathcal{G}_\ell^{R-}(k;r,r')$. The value of the integral appearing in (15) for the wave number k *on* the real axis must be defined as a limit in k. The limit from above is used by Newton [16] to define the *outgoing-wave resolvent* $\mathcal{G}_\ell^{(+)}$ if $\mathrm{Re}(k)$ is positive, the *incoming-wave resolvent* $\mathcal{G}_\ell^{(-)}$ if $\mathrm{Re}(k)$ is negative. This limit is conveniently obtained by deforming the integration path downwards so that the pole at $q = \kappa$, where κ is real, is circumvented by a semicircle with infinitesimal radius. Since the pole is simple, we get in a well-known way

$$\mathcal{G}_\ell^{R+}(\kappa;r,r') = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{\kappa-q} - \frac{i}{\kappa}\psi_\ell(\kappa,r)\psi_\ell^*(\kappa,r') + \Sigma_b,$$

i.e., a principal value integral and a δ function contribution. If one instead takes the limit from *below* the real axis, one obtains

$$\mathcal{G}_\ell^{R-}(\kappa;r,r') = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{\kappa-q} + \frac{i}{\kappa}\psi_\ell(\kappa,r)\psi_\ell^*(\kappa,r') + \Sigma_b,$$

from which one gets the discontinuity over the branch cut

$$\mathcal{G}_\ell^{R-}(\kappa;r,r') - \mathcal{G}_\ell^{R+}(\kappa;r,r') = \frac{2i}{\kappa}\psi_\ell(\kappa,r)\psi_\ell^*(\kappa,r'). \quad (17)$$

The basic definition of $\mathcal{G}_\ell(k;r,r')$, Eq. (12) yields, on the other hand,

$$\mathcal{G}_\ell(-\kappa;r,r') - \mathcal{G}_\ell(\kappa;r,r') = (-1)^{\ell+1}\kappa^\ell\varphi_\ell(\kappa,r_<)(-1)^\ell\left\{\frac{f_\ell(\kappa,r_>)}{f_\ell(\kappa)} - (-1)^\ell\frac{f_\ell(-\kappa,r_>)}{f_\ell(-\kappa)}\right\} = \frac{2i\kappa^{2\ell+2}}{\kappa}\frac{\varphi_\ell(\kappa,r_<)\varphi_\ell(\kappa,r_>)}{f_\ell(-\kappa)f_\ell(\kappa)}, \quad (18)$$

where we have used the general relation between the regular solution $\varphi_\ell(k,r)$ and the irregular solutions $f_\ell(\pm k,r)$ quoted in the Appendix, Eq. (A1). This relation is symmetric in r and r' which may now replace $r_<$ and $r_>$, and we may further introduce the scattering states $\psi_\ell(\kappa,r)$ using Eq. (1). The discontinuity over the branch cut obtained in Eq. (17) thus turns out to be identical to the difference $\mathcal{G}_\ell(-\kappa;r,r') - \mathcal{G}_\ell(\kappa;r,r')$ which confirms the conclusion that, with equal signs for $\mathrm{Re}(k) > 0$,

$$\mathcal{G}_\ell^{R\pm}(k;r,r') = \mathcal{G}_\ell(\pm k;r,r')$$

in the upper and lower half k planes, respectively. This shows the range of validity of Eq. (15) as an eigenfunction expansion.

A. Resonant state expansion of the resolvent

We will now attempt to extend the range of the expansion (15) for $\mathcal{G}_\ell^{(+)}(k)$ so as to include also resonant states using a procedure similar to the one described in Sec. II, viz., by deforming the integration contour from R to W (see Fig. 2). This amounts to constructing an analytic continuation of the function defined in the upper k half-plane by the integrals in (15) down into the upper part of the lower half-plane by deforming the branch cut. The contour W passes *below* the resonance poles selected and retains the symmetry with respect to reflection in the imaginary axis (if q is on W then so is $-q^*$). This symmetry is different from the *inversion symmetry* (invariance under $q \to -q$) characterizing the continuum of a properly derived *completeness* relation. Therefore, since the resolvent operator is *not* inversion symmetric but satisfies (14) it is necessary to derive its resonant state expansion directly without using the completeness relations. Let $\mathbf{W}$ be the domain consisting of the upper half k plane extended down to and including W. We then get, provided the integrand, apart from the poles at k_n and $-k_n^*$, is analytic in a strip containing W and R,

$$\frac{1}{\pi}\int_W\frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k-q} + \frac{1}{\pi}\int_\infty^{-\infty}\frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k-q} = 2i\sum_{k_n\in\mathbf{W}\setminus\mathbf{R}}\mathrm{Res}_{k=k_n},$$

since the two integrals in the left member obviously are

[3]If the Jost function $f_\ell(-k)$ happens to have a zero for $k = 0$, special treatment may be necessary; see further Newton [16].

together taken over a closed path that encloses the domain denoted by $\mathbf{W}\backslash\mathbf{R}$. [A more cautious procedure would be to multiply Eq. (15) by sufficiently regular "test" functions $h_1(r)$ and $h_2(r')$, then integrate over r and r', and finally replace the test functions by δ functions. The result is the same.] Using Eqs. (6a) and (6d) for the residues of $\psi_\ell\psi_\ell^*$ and remembering the factor $1/[q(k-q)]$ we easily get

$$\frac{1}{\pi}\int_W \frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k-q} = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k-q} + \sum_{k_n\in\mathbf{W}\backslash\mathbf{R}} u_n(r)\tilde{u}_n^*(r')\left(-\frac{1}{2k_n(k-k_n)}\right).$$

It is then natural to define, for all $k\in\mathbf{W}$,

$$\mathcal{G}_\ell^W(k;r,r') = \frac{1}{\pi}\int_W \frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k-q} + \Sigma_b + \sum_{k_n\in\mathbf{W}\backslash\mathbf{R}} \frac{u_n(r)\tilde{u}_n^*(r')}{2k_n(k-k_n)}. \quad (19)$$

In the domain $\mathbf{W}$ above and including W and the real axis, this function has the same analytic properties as $\mathcal{G}_\ell(k;r,r')$ defined by Eq. (12) and the same symmetry with respect to the substitution $k\to -k^*$. Applied to test functions, (19) is equivalent to $\mathcal{G}_\ell^{R+}(k;r,r')$ by Cauchy's theorem and we thus consider it as the proper resonant state expansion of the function $\mathcal{G}_\ell^{R+}(k;r,r')$ and thereby (within $\mathbf{W}$) of the resolvent $\mathcal{G}_\ell(k;r,r')$. In a similar manner we may obviously continue the function $\mathcal{G}_\ell^{R-}(k;r,r')$ defined in the lower half-plane by Eq. (15) upwards to a curve W^* which is the mirror image of W with respect to the real k axis, thereby obtaining a resonant state expansion $\mathcal{G}_\ell^{W^*}(k;r,r')$ of $\mathcal{G}_\ell(-k;r,r')$ valid in the domain $\mathbf{W}^*$ below and including W^* and the real k axis. (Notice that the asterix in the superscript of the symbol $\mathcal{G}$ is a superscript on W with no direct significance for $\mathcal{G}$.) Just as in the case of wave function expansions, we should interpret the functions defined by the expansion as representatives with respect to different sets of basis functions specified by W (or W^*) and R, respectively, and with different ranges of validity. We observe that the set of discrete terms in the resonant state expansion (19) obtained in this way contains a finite subset of the terms in the Mittag-Leffler version of the resolvent used, e.g., in Refs. [9, 10]. We also see that if $k\in\mathbf{W}$ then $-k\in\mathbf{W}^*$ and we may readily show that $\mathcal{G}_\ell^{W^*}(k;r,r') = \mathcal{G}_\ell^W(-k;r,r')$. Note, however, that if $W\neq R$, then there exist $k\in\mathbf{W}$ such that also $-k\in\mathbf{W}$.

There seems to be no compelling reason why we should draw the contour W so that it goes through the origin $k=0$ except that this point is the branch point of the physical operator. (The latter fact does not seem to have any palpable numerical consequences, though.) By drawing the contour in a U-shaped fashion so that it passes below the poles corresponding to the antibound states ($k_a=-i\gamma_a$ with $\gamma_a>0$), the sum Σ_b would also include the antibound states and have the same denominators as the sum over the resonance terms. Such a contour has been suggested by Romo [15] for use also in completeness relations. For that purpose the U-shaped contour may be questionable since it is not inversion symmetric. However, with respect to expansions of the *resolvent*, the U contour has the reflection symmetry with respect to the imaginary axis that is required by the symmetries of this operator. Equation (19) with a domain $\mathbf{U}$ consisting of the upper half k plane extended down to and including U then gives

$$\mathcal{G}_\ell^U(k;r,r') = \frac{1}{\pi}\int_U \frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k-q} + \sum_{k_n\in\mathbf{U}} \frac{u_n(r)\tilde{u}_n^*(r')}{2k_n(k-k_n)}. \quad (20)$$

This is equivalent to Romo's result in Ref. [15], i.e., of the form known from Mittag-Leffler theory but without the restriction to finite-range interactions.

If we had not restricted ourselves to contours that are symmetric with respect to reflection in the imaginary k axis, we could also have derived in the same way (i.e., by direct analytic continuation) the expansion

$$\mathcal{G}_\ell^L(k;r,r') = \frac{1}{\pi}\int_L \frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k-q} + \sum_{k_n\in\mathbf{L}} \frac{u_n(r)\tilde{u}_n^*(r')}{k^2-k_n^2}, \quad (21)$$

where $\mathbf{L}$ is the domain consisting of the k plane above and including the L contour. This expansion could also have been derived as in [6] by using the completeness relation (9). The point to observe is that the integral and the discrete part of this latter expansion do not *separately* have the symmetry (14) whereas this symmetry is valid for both types of terms in the expansions $\mathcal{G}_\ell^W(k)$ and $\mathcal{G}_\ell^U(k)$. Taking the difference between Eqs. (21) and (20) we get an expression that by Cauchy's theorem is identically 0 (this follows, of course, from the construction of the expansions). Both types of expansions are therefore valid *if the continuum term is kept.*

The resonant state expansions have the advantage that they give simple expressions for the behavior of the resolvent in the vicinity of its poles. It is therefore convenient to introduce the notation $G_\ell^C(k)$ with $C=L$, W, or U to denote the approximations obtained by neglecting the integrals in (21), (19), and (20) respectively. Then these expansions can be summarized in

$$\mathcal{G}_\ell^C(k;r,r') = \frac{1}{\pi}\int_C \frac{dq}{q}\frac{\psi_\ell(q,r)\psi_\ell^*(q^*,r')}{k-q} + G_\ell^C(k;r,r')\ , \quad C=L,W,U.$$

We can already note that the approximation $G_\ell^L(k)$ does not have the symmetry property (14) and that the approximations $G_\ell^L(k)$ and $G_\ell^W(k)$ have false poles at $k = -k_b$ and $G_\ell^L(k)$ also at $k = -k_d$. This means that they cannot fully represent the resolvent (the integral part is still of importance since it contains the corrective contributions) and in some calculations, e.g., [22], the relative error can have a magnitude of order unity. There might nevertheless be cases for which these objections are less important. Thus the only integral which might be negligibly small or even vanish exactly is the one over the U contour. This is supported by Mittag-Leffler theory for the case of a finite-range potential.

In Ref. [12] the approximations $G_\ell^L(k)$ and $G_\ell^U(k)$ were denoted "Berggren" and "Mittag-Leffler" expansions, respectively, since they were considered to have been derived using different theories. The notation chosen in the present paper is meant to emphasize that the different expansions can indeed be obtained by the same method starting from the results of Newton [16]. In view of this it is not surprising that the so-called "Mittag-Leffler expansion" might be valid also when the Coulomb potential is included, which was another major conclusion of Ref. [12].

B. Numerical illustrations

To study the properties of different (approximate) expansions of the resolvent we consider some average over the radial coordinates rather than the value at some specific points. One such quantity is the partial wave S-matrix element $S_\ell(k) = 1 - 2T_\ell(k)/ik$, which we express in terms of the partial elastic scattering amplitude (transition matrix element)

$$T_\ell(k) = \langle\psi_\ell^0(k)|V|\psi_\ell(k)\rangle$$
$$= \langle\psi_\ell^0(k)|V|\psi_\ell^0(k)\rangle + \langle\psi_\ell^0(k)|V\mathcal{G}_\ell(k)V|\psi_\ell^0(k)\rangle. \quad (22)$$

Here $\psi_\ell^0(k,r)$ is the free wave function and $\psi_\ell(k,r)$ the scattering wave function. We have introduced the resolvent $\mathcal{G}_\ell(k)$ by expressing ψ_ℓ in terms of ψ_ℓ^0 through the formal solution of the Lippmann-Schwinger equation. Bang *et al.* [23] studied the pole expansion of $S_\ell(k)$ using Mittag-Leffler theory finding that, for cutoff potentials, the expansion obtained is the same as using $\mathcal{G}_\ell(k) \approx G_\ell^U(k)$. Their conclusion was that the expansion is convergent also without using the possibility of adding an entire function to the sum.

Another resolvent-dependent quantity, the single-particle response function

$$R_\ell(k) = \langle f_\ell|\mathcal{G}_\ell(k)|f_\ell\rangle$$
$$= \int f_\ell(r)\mathcal{G}_\ell(k;r,r')f_\ell(r')dr\,dr', \quad (23)$$

where f_ℓ is the form factor associated with a multipole operator, was used in [12] to compare the approximations $\mathcal{G}_\ell(k) \approx G_\ell^L(k)$ and $\mathcal{G}_\ell(k) \approx G_\ell^U(k)$. The conclusions were that the two expansions have similar behavior (as functions of energy) except at threshold, i.e., as $k \to 0$, and that only one term is needed to reproduce the exact response function in the resonant regions while two terms might suffice for energies between resonances.

Using the approximation $\mathcal{G}_\ell(k) \approx G_\ell^U(k)$ we obtain an expansion of the response function of the form

$$R_\ell^U(k) = \sum_{k_n \in \mathrm{U}} \frac{\rho_n}{2k_n(k-k_n)}, \quad \rho_n = \langle\tilde{u}_n|f_\ell\rangle^2,$$

where the numerator has no k dependence. This makes it obvious that if the expansion is valid then we might need only the states immediately below and above the energy considered to reproduce the exact response function between resonances. This should hold at least if the other states are so far away that their contribution to the background is small, which might not be the case in the low-energy region. The expansion of the elastic amplitude instead looks like

$$T_\ell^U(k) = \langle\psi_\ell^0(k)|V|\psi_\ell^0(k)\rangle + \sum_{k_n \in \mathrm{U}} \frac{\tau_n(k)}{2k_n(k-k_n)},$$
$$\tau_n(k) \equiv \langle\tilde{u}_n|V|\psi_\ell^0(k)\rangle^2,$$

where now also the numerator is k dependent. This means that each term might give a contribution over a larger interval than suggested by the denominator and interfere stronger with the background due to the other terms. We therefore expect that several states might be needed to reproduce the nonresonant behavior.

1. Elastic scattering amplitude

In order to check also the validity of the approximation $\mathcal{G}_\ell(k) \approx G_\ell^W(k)$ we calculate the partial elastic amplitude $T_\ell(k)$ for the same potential (a square well of radius $R_0 = 7$ fm and depth $-V_0 = -45$ MeV), angular momentum ($\ell = 4$), and energy range ($E < 50$ MeV) including the same states as in Figs. 2 and 3 of [12]. Due to the analytical properties of the square well model we also have the possibility to check the convergence when including a large number of resonances and to see the influence of antibound states and virtual resonances. The potential in these studies gives rise to one sharp and one virtual resonance. (We note in passing that it also has more antibound states than bound states, i.e., a deviation from the simple picture of pole trajectories presented in [24].) We give in Table I the eigenvalues of the states with lowest

TABLE I. Eigenvalues with Re$E < 100$ MeV and angular momentum $\ell = 4$, for the square well potential with $R_0 = 7$ fm and $V_0 = 45$ MeV. The form of the energy denominator used in the approximations with subscripts L, W, and U is indicated by + for $k^2 - {k_n}^2$, × for $2k_n(k-k_n)$. An $*$ is added if also the term corresponding to $\tilde{k}_n$ is included.

k_n (fm^{-1})		Energy (MeV)		L	W	U
Re	Im	Re	Im			
0.000	+1.016	−21.587		+	+	×
0.000	−0.652	−8.896				×
0.000	−0.441	−4.073				×
0.307	−0.334	−0.354	−4.293	+	×*	×*
0.217	−0.0002	0.988	−0.002	+	×*	×*
1.212	−0.156	30.20	−7.931	+	×*	×*
1.865	−0.191	71.97	−14.93	+	×*	×*

energy.

In Fig. 3 we show separately the real and imaginary parts of $T_\ell(k)$ and the approximations $T_\ell^C(k) = \langle\psi_\ell^0(k)|V[1+G_\ell^C(k)V]|\psi_\ell^0(k)\rangle$, with $C = L$, W, and U. [In order to make the sharp resonance visible we have actually plotted the real and imaginary parts of $T_\ell^*(k)/k$.] The curves denoted $N_{\rm res} = 4$ include only the states of Table I. We see that it is only the imaginary part that can be reasonably well approximated by as few as four resonances and only by $T_\ell^U(k)$. This still might be reassuring since only $-{\rm Im}T_\ell(k)$ is needed to calculate the partial cross section, but the difficulty with reproducing the real part is important for understanding the convergence of resonant state expansions. We have therefore included approximations with a large number of resonances ($N_{\rm res} = 175$). We may conclude that ultimately also the real part will be well reproduced by $T_\ell^U(k)$. However, the approximations based on $G_\ell^L(k)$ and $G_\ell^W(k)$ do *not* improve when more resonances are included. (Note also that they would give a negative cross section at some energies.)

We may also remark that all the terms in the $N_{\rm res} = 4$ expansions give contributions of the same order of magnitude, which means that none of these terms is negligible. The very striking difference between the $T_\ell^W(k)$ and $T_\ell^U(k)$ approximations is due entirely to the presence of antibound states and the absence of false bound state poles in the latter form of expansion. Not even the virtual resonance can be neglected in $T_\ell^U(k)$ without destroying the quality of the fit.

In contradiction to what was stated in connection with the expansions of the response function in [12] we must conclude that the expansions of the partial elastic amplitude based on $G_\ell^L(k)$ and $G_\ell^U(k)$ do *not* have similar behavior (except at threshold) and that several states might be needed to reproduce nonresonant behavior.

2. Convergence aspects

To see how the approximation improves when one includes more terms in $T_\ell^U(k)$, we show in Fig. 4 the logarithm of the relative error $\log_{10}|(t^U - t)/t|$ as a function of $N_{\rm res}$. Here t and t^U are either the real or the imaginary parts of $T_\ell(k)$ and $T_\ell^U(k)$, respectively. The dips in these curves occur when the approximation crosses the exact amplitude in Fig. 3. These crossings move when we include more terms (as will be seen also in Fig. 5). Some of these dips will be filled in as the approximate curve approaches the exact one. The peaks in the curves for the error of the real part in Fig. 4 are due to the zeros of the

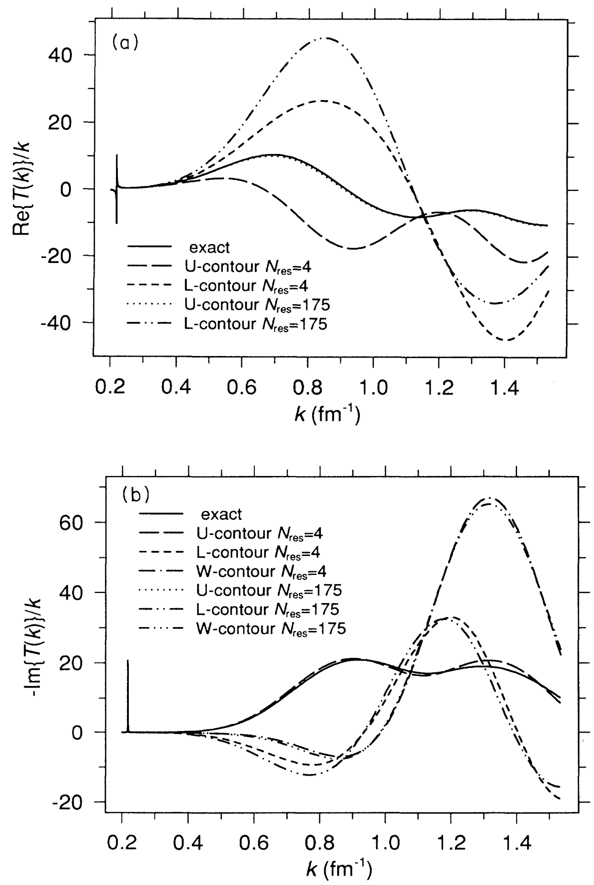

FIG. 3. Real and imaginary parts of $T_\ell^*(k)/k$. The real parts of $T_\ell^L(k)$ and $T_\ell^W(k)$ are equal. For $N_{\rm res} = 175$ the imaginary part of $T_\ell^U(k)$ coincides with the exact one.

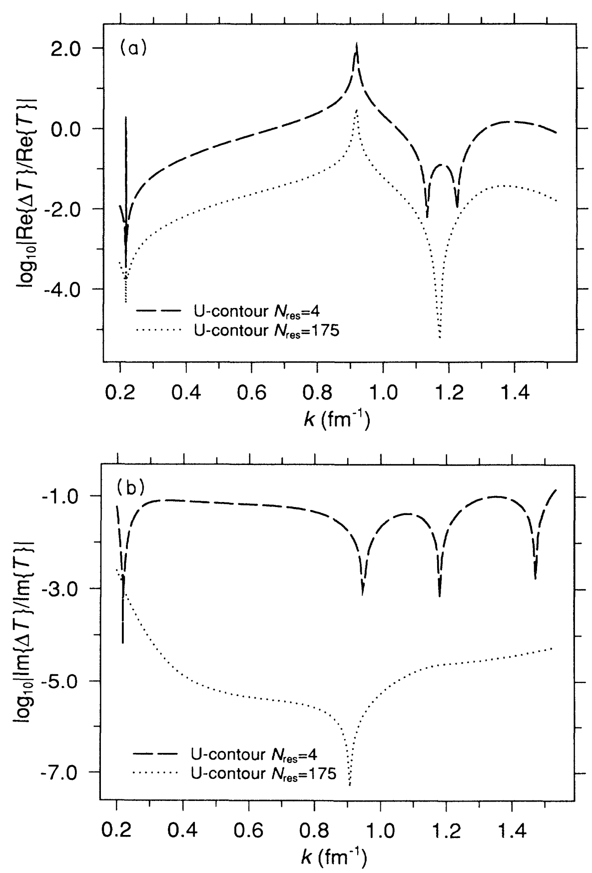

FIG. 4. Logarithm of the relative error of the real and imaginary parts of $T_\ell^U(k)$ of Fig. 3.

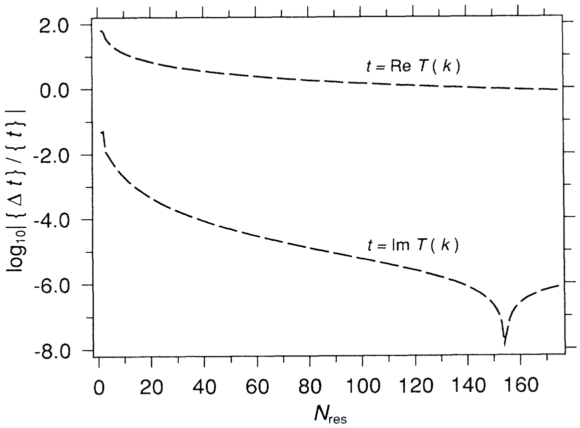

FIG. 5. Logarithm of the relative error of the real and imaginary parts of $T_\ell^U(k)$ as functions of the number $N_{\rm res}$ of resonances included in the expansion. The amplitudes are evaluated at $k = 0.926\,43$. (The energy of the 175th resonance is 131 GeV.)

exact amplitude which will enhance any small but finite deviation. (There are no zeros in the imaginary part of the elastic amplitude since there is only one bound state with $\ell = 4$ in this potential.)

To see the convergence as more terms are included we show in Fig. 5 the relative error at a fixed k value as function of the number of resonances included. (Only the decaying resonances are counted although the corresponding capturing states are included in the U expansion.) We see that, as indicated also in Fig. 4, the imaginary part converges faster than the real part. To produce Fig. 5 we selected a k value near the peak of Fig. 4, i.e., a point where the real part of the exact amplitude is zero and thus the relative error is inconvenient as a measure of accuracy. Although the relative error at $N_{\rm res} = 175$ is 82%, the rate of convergence is the same as for other k values.

3. Threshold behavior

The threshold behavior ($k \to 0$) of $T_\ell(k)$ is determined by the k dependence of the scattering functions. This is the same in the approximations $T_\ell^C(k)$ so that the $k^{2(\ell+1)}$ behavior is reproduced. Since the single-particle response function is an average of the resolvent weighted by real k-independent functions it should have the symmetry (14), i.e., $R_\ell(-k^*) = R_\ell^*(k)$. Consequently ${\rm Im}R_\ell(k) \to 0$, $k \to 0$, and ${\rm Im}R_\ell(i\gamma) = 0$, γ real. The imaginary part of the response function is the single-particle strength function which should vanish for negative energies. Since the approximation $G_\ell^L(k)$ does not have the symmetry (14) it is obvious that it will lead to a strength function, $-{\rm Im}R_\ell^L(k)$, that does not vanish below threshold. This is exactly what was observed in [12]. Despite the lack of correct symmetry and the inclusion of the false poles, the approximation $R_\ell^L(k)$ seems to work rather well also far away from threshold, but then, on the other hand, the response function is a quantity that shows resonant behavior even for the broad resonances.

IV. CONCLUSIONS

For the purpose of developing perturbation theories utilizing resonant states a relevant problem is how to expand the resolvent. We have here pointed to the fact that the symmetry properties of the resolvent are more restrictive than those of the projection operators involved in ordinary resonant state expansions. This leads to an expression for the contribution of a resonant state to the *resolvent* that is identical to that of the Mittag-Leffler theory [15] and different from the forms obtained by directly applying the completeness relations [6] to the resolvent operator $1/(E-H)$. As shown by Romo [15, 22], the spurious poles introduced in the latter case impair seriously the convergence of perturbation expansions. Therefore, if continuum contributions could be completely ignored, the pure Mittag-Leffler expansion would seem to be preferable. The Mittag-Leffler theory is, however, based on still stronger conditions than those we imposed on the test functions, namely, the strict vanishing of the potential outside a finite range. Although such a restriction might appear acceptable from the practical point of view, it excludes in principle most of the interactions generally employed in nuclear physics. The resonant state expansions are not restricted in this respect and therefore provide a more useful tool for investigations in the theory of nuclear structure and nuclear reactions. It is therefore gratifying that the method which we here describe, when applied to the resolvent with due regard to the symmetries of this operator, indeed does yield the Mittag-Leffler expressions for the discrete terms of the expansion and that in the finite-range case the continuum contribution can be calculated and shown to vanish.

In this work we have thus found (in contradiction to Ref. [12]) that the so-called "Berggren expansion" of the resolvent (21) is unreliable and that the proper expansion is of the Mittag-Leffler form (20). Although the completeness relation and the expansion of the resolvent are intimately related, the criteria for the choice of contour in the completeness relation are not the same as for the resolvent. The set of discrete states in the form (9) of the completeness relation seems to be the natural extension of the bound single-particle basis while the Mittag-Leffler form (11) has a problem with overcompleteness and the interpretation of the virtual states. The usefulness of the form (10) is a very problematic question, since it is superseded by the Mittag-Leffler expansion (11) inside the range of the potential. There is no reason to doubt the validity of (10) as a completeness relation. The continuum contribution may for $r < R$ be calculated resulting in a sum of discrete terms which merge with the resonant terms so as to give (11). These matters are under investigation [21].

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APPENDIX: DERIVATIVE OF THE JOST FUNCTION

The following considerations are based on (and to some extent are quotations from) Newton's paper [16], Sec. IV, generalizing Newton's result to hold also for resonant states. The regular solution $\varphi_\ell(k,r)$ of the radial Schrödinger equation corresponding to the orbital angular momentum $\hbar\ell$ can be expressed in terms of the irregular Jost solutions $f_\ell(k,r)$ defined such that

$$\exp(ikr)f_\ell(k,r) \sim i^\ell, \qquad r\to\infty.$$

According to Newton [16]

$$\varphi_\ell(k,r) = \frac{1}{2}ik^{-\ell-1} \times\{f_\ell(-k)f_\ell(k,r) - (-1)^\ell f_\ell(k)f_\ell(-k,r)\}. \tag{A1}$$

As the radial Schrödinger equation contains no first-order derivative, the Wronski determinant of any two arbitrary solutions is constant and may be determined from the asymptotic behavior:

$$W[f_\ell(k,r), f_\ell(-k,r)] = (-1)^\ell 2ik,$$

where

$$W[f,g] \equiv fg' - f'g.$$

Equation (A1) gives

$$f_\ell(k) = k^\ell W[f_\ell(k,r),\varphi_\ell(k,r)].$$

Using the notation $\partial_k \equiv \partial/\partial k$ we get by differentiation

$$\begin{aligned}\frac{df_\ell(k)}{dk} &= \ell k^{\ell-1}W[f_\ell(k,r),\varphi_\ell(k,r)] \\ &\quad +k^\ell W[\partial_k f_\ell(k,r),\varphi_\ell(k,r)] \\ &\quad +k^\ell W[f_\ell(k,r),\partial_k\varphi_\ell(k,r)].\end{aligned} \tag{A2}$$

If $k = k_0$ is such that $f_\ell(k_0) = 0$, then $\varphi_\ell(k_0,r) = \zeta f_\ell(k_0,r)$ and obviously $W[f_\ell,\varphi_\ell] = 0$. Then (note that the definition of ζ yields the inverse of Newton's coefficient c)

$$\zeta = \frac{if_\ell(-k_0)}{2k_0^{\ell+1}}. \tag{A3}$$

Equation (A2) gives, for this value of k,

$$\begin{aligned}\left.\frac{df_\ell(k)}{dk}\right|_{k=k_0} &= k_0^\ell\zeta W[\partial_{k_0}f_\ell(k_0,r), f_\ell(k_0,r)] \\ &\quad +(k_0^\ell/\zeta)W[\varphi_\ell(k_0,r),\partial_{k_0}\varphi_\ell(k_0,r)].\end{aligned} \tag{A4}$$

The Wronski determinants in the right member may be calculated from

$$\frac{dW[f_\ell(k,r),f_\ell(k',r)]}{dr} = (k^2-k'^2)f_\ell(k,r)f_\ell(k',r),$$

which is easily deduced from the wave equations for $f_\ell(k,r)$ and $f_\ell(k',r)$. Analogous equations hold for $\varphi_\ell(k,r)$ and $\varphi_\ell(k',r)$. Differentiate with respect to k and then put $k'=k$ so as to obtain

$$\frac{dW[\partial_k f_\ell(k,r),f_\ell(k,r)]}{dr} = 2kf_\ell(k,r)^2,$$

$$\frac{dW[\partial_k\varphi_\ell(k,r),\varphi_\ell(k,r)]}{dr} = 2k\varphi_\ell(k,r)^2.$$

With the usual conditions on k the first equation may be integrated, if necessary using regularization, from r to infinity, whereas the second equation can be integrated without problems from 0 to r:

$$W[\partial_k f_\ell(k,r'),f_\ell(k,r')]|_{r'=\infty} - W[\partial_k f_\ell(k,r),f_\ell(k,r)] = 2k\int_r^\infty dr' f_\ell(k,r')^2,$$

$$W[\partial_k\varphi_\ell(k,r),\varphi_\ell(k,r)] - W[\partial_k\varphi_\ell(k,r'),\varphi_\ell(k,r')]|_{r'=0} = 2k\int_0^r dr'\varphi_\ell(k,r')^2.$$

The value of $W[\partial_k f_\ell(k,r'),f_\ell(k,r')]_{r'=\infty}$ should be interpreted as a regularized limit [4] and may then be put equal to 0. Furthermore, $W[\partial_k\varphi_\ell(k,r'),\varphi_\ell(k,r')]_{r'=0} = 0$ according to the boundary condition

$$\varphi_\ell(k,r) \sim r^{\ell+1}/(2\ell+1)!!$$

and then

$$W[\partial_k f_\ell(k,r),f_\ell(k,r)] = -2k\int_r^\infty dr' f_\ell(k,r')^2,$$

$$W[\partial_k\varphi_\ell(k,r),\varphi_\ell(k,r)] = 2k\int_0^r dr'\varphi_\ell(k,r')^2.$$

For $k = k_0$ these results are substituted into Eq. (A4) giving

$$\begin{aligned}\left.\frac{df_\ell(k)}{dk}\right|_{k=k_0} &= -2k_0^{\ell+1}\zeta\int_r^\infty dr' f_\ell(k_0,r')^2 \\ &\quad -\frac{2k_0^{\ell+1}}{\zeta}\int_0^r dr'\varphi_\ell(k_0,r')^2 \\ &= -\frac{2k_0^{\ell+1}}{\zeta}\int_0^\infty dr'\varphi_\ell(k_0,r')^2.\end{aligned} \tag{A5}$$

Inserting, finally, the proper value of ζ found above, Eq. (A3), we obtain Eq. (5) of Sec. II.

[4] With a Gaussian convergence factor $\exp(-\epsilon r^2)$ the regularized limit [6] of a function $y(r)$ is defined by $\lim_{r\to\infty} y(r) = \lim_{\epsilon\to 0}\int_0^\infty 2\epsilon x\,dx\,\exp(-\epsilon x^2)y(x)dx$. This yields 0 for $y(r) = r\exp(-2ikr)$ if $\mathrm{Im}(k) \le \mathrm{Re}(k)$.

[1] G. Gamow, Z. Phys. **51**, 204 (1928).
[2] A. F. J. Siegert, Phys. Rev. **56**, 750 (1939).
[3] J. Humblet and L. Rosenfeld, Nucl. Phys. **26**, 529 (1961).
[4] Ya. B. Zel'dovich, Zh. Eksp. Teor. Fiz. **39**, 776 (1960) [Sov. Phys. JETP **12**, 542 (1961)].
[5] N. Hokkyo, Prog. Theor. Phys. **33**, 1116 (1965).
[6] T. Berggren, Nucl. Phys. **A109**, 265 (1968).
[7] W. J. Romo, Nucl. Phys. **A116**, 617 (1968).
[8] C. Mahaux and H. A. Weidenmüller, *Shell Model Approach to Nuclear Reactions* (North-Holland, Amsterdam, 1969).
[9] T. Vertse, P. Curutchet, O. Civitarese, L. S. Ferreira, and R. J. Liotta, Phys. Rev. C **37**, 876 (1988).
[10] P. Curutchet, T. Vertse, and R. J. Liotta, Phys. Rev. C **39**, 1020 (1989).
[11] T. Vertse, P. Curutchet, and R. J. Liotta, in *Resonances*, edited by E. Brändas and N. Elander, Lecture Notes in Physics Vol. 325 (Springer Verlag, New York, 1989), p. 179.
[12] T. Vertse, P. Curutchet, and R. J. Liotta, Phys. Rev. C **42**, 2605 (1990).
[13] T. Vertse, P. Curutchet, R.J. Liotta, J. Bang, and N. Van Giai, Phys. Lett. B **264**, 1 (1991).
[14] T. Berggren, Nucl. Phys. **A389**, 261 (1982).
[15] W. J. Romo, Nucl. Phys. **A398**, 525 (1983).
[16] R. Newton, J. Math. Phys **1**, 319 (1960).
[17] R. Jost, Helv. Phys. Acta **20**, 256 (1947).
[18] B. Gyarmati and T. Vertse, Nucl. Phys. **A160**, 523 (1971).
[19] J. Bang, F. A. Gareev, M. H. Gizzatkulov, and S. A. Gonchanov, Nucl. Phys. **A309**, 381 (1978).
[20] W. J. Romo, J. Math. Phys **21**, 311 (1980).
[21] P. Lind (submitted to Phys. Rev. C).
[22] W. J. Romo, Nucl. Phys. **A142**, 300 (1970).
[23] J. Bang, S. N. Ershov, F. A. Gareev, and G. S. Kazacha, Nucl. Phys. **A339**, 89 (1980).
[24] H. M. Nussenzveig, Nucl. Phys. **11**, 499 (1959).