Completeness relations and resonant state expansions

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(Received 23 December 1992)

The completeness properties of the discrete set of bound states, virtual states, and resonant states characterizing the system of a single nonrelativistic particle moving in a central cutoff potential are investigated. We do not limit ourselves to the restricted form of completeness that can be obtained from Mittag-Leffler theory in this case. Instead we will make use of the information contained in the asymptotic behavior of the discrete states to get a new approach to the question of eventual overcompleteness. Using the theory of analytic functions we derive a number of completeness relations in terms of discrete states and complex continuum states and give some criteria for how to use them to form resonant state expansions of functions, matrix elements, and Green's functions. In cases where the integral contribution vanishes, the discrete part of the expansions is of the same form as that given by Mittag-Leffler theory but with regularized inner products. We also consider the possibility of using the discrete states as basis in a matrix representation.

PACS number(s): 24.30.−v, 03.65.Nk

I. INTRODUCTION

Resonance (or *Gamow*) wave functions were introduced long ago into nuclear physics to describe decaying states [1]. Many methods have been developed for how to normalize these seemingly divergent functions and use them to calculate inner products [2–5]. By associating them with poles of the S matrix they could be treated as eigenstates [6] and used to form pole expansions of the S matrix and convenient parametrizations of cross sections near resonances [7]. The most important step forward in the theory of resonant state expansions must have been the derivation of completeness relations in terms of bound states and resonances [4]. This eigenfunction theory suggests the possibility to use the set of bound states and decaying resonances as a basis also in nuclear structure calculations.

It is a fact that the nuclear potentials can be truncated with reasonable accuracy at a distance of a few nuclear radii and this is also a necessity in all numerical calculations. In this paper we therefore consider only a *cutoff* potential

$$V(r) = 0\ ,\ r > R_C. \tag{1}$$

One can then use the pole expansions of Mittag-Leffler theory to derive other "completeness relations," which are valid (although the basis functions are linearly dependent) in this finite radial space. There has been much debate over the years between the advocates of the two theories, but we would now like to think of the relations of the Mittag-Leffler theory as a special case of the more general eigenfunction theory, which is valid in the infinite radial space.

Much attention has been paid to the properties of the resonance states themselves but not so much to the fact that they are included in a completeness relation (and what that means). In this paper we will investigate and illustrate how to use complete sets of generalized eigenfunctions to obtain expansions of functions, matrix elements, and Green's functions and how to solve exactly a perturbation problem even for the eigenvalues of resonances and antibound states. The aim here is to summarize and unify various relations and formulas and show the power of these eigenfunction expansions. Most important is then to be able to use these expansions (just as an ordinary eigenfunction expansion) to calculate (numerically) quantities that do not necessarily show resonant behavior and can be calculated exactly.

We make here no mathematical proof of convergence of the expansions obtained. Instead we have checked every statement by a numerical calculation where the exact value is known or calculable with other methods. This was considered necessary because there has been too much speculation in this area over the years that has not been verified by relevant calculations. Since we would like to apply our theory to nuclear processes in the continuum but demand high numerical accuracy in our investigations, we choose to use a square well potential

$$V(r) = \begin{cases} -V_\square, r < R_\square \\ 0, \quad r > R_\square \end{cases} \tag{2}$$

to generate our basis functions. By choosing as the basis neutral S-wave states, we include no sharp resonances and thus the completeness properties can be investigated without having dominating contributions from one single state. If we choose the radius of the square well $R_\square$ similar to that of a heavy nucleus, we get a realistic behavior of the low-energy spectrum (independent of the depth of the well). The distribution of the high-energy resonances, on the other hand, depends on the cutoff radius R_C, but these states are used only to represent the continuum.

II. A COMPLETE SET OF FUNCTIONS

In quantum mechanics (e.g., [8]) we usually assume the existence of a complete set $\{|n\rangle\}$ of orthonormal, $\langle m|n\rangle = \delta_{mn}$, (eigen)functions in terms of which we can

expand any function belonging to a certain class of functions (obeying some certain conditions)

$$|\Phi\rangle = \sum_n c_n |n\rangle, \tag{3}$$

where $c_n = \langle n|\Phi\rangle$. Since the set is complete we have the *completeness relation*

$$\langle\Phi|\Phi\rangle = \sum_n |c_n|^2 \tag{4}$$

and the *closure relation*

$$\delta(r-r') = \sum_n u_n(r) u_n^*(r'), \tag{5}$$

which we can write more abstractly as a *projection operator* (or *resolution of unity*)

$$\mathbb{1} = \sum_n |n\rangle\langle n|. \tag{6}$$

The completeness properties are so fundamental and important that the name completeness relation often is used also for the relations (5) and (6). This is traditional in the theory of resonant state expansions and used also in this paper.

It is because of the completeness properties of eigenfunctions that we can transform functions

$$|\Phi\rangle \to \sum_n c_n |n\rangle \ , \ c_n = \langle n|\Phi\rangle,$$

operators

$$\mathcal{A} \to \sum_{m,n} |m\rangle A_{mn} \langle n|,$$

and (differential) equations

$$\mathcal{D}|\Phi\rangle = 0 \to \sum_{m,n} D_{mn} c_n |m\rangle = 0$$

into a matrix representation where often the equations are easier to solve and scalar quantities easier to calculate and interpret.

In this work on completeness relations we do not stop with a convergent expansion of a matrix element like

$$\langle\Phi_1|AB|\Phi_2\rangle = \langle\Phi_1|A\mathbb{1}B|\Phi_2\rangle = \sum_n \langle\Phi_1|A|n\rangle\langle n|B|\Phi_2\rangle$$

but we will also study the conditions under which a resolution of unity (6) is really a projection operator, a case which is not obvious when including the resonant states. This latter property is essential for an expansion like

$$\begin{aligned}\langle\Phi_1|AB|\Phi_2\rangle &= \langle\Phi_1|\mathbb{1}AB\mathbb{1}|\Phi_2\rangle \\ &= \sum_{m,n} \langle\Phi_1|m\rangle\langle m|AB|n\rangle\langle n|\Phi_2\rangle\end{aligned}$$

and for the use of a complete set of discrete states as an unperturbed basis to solve a matrix equation for the properties of the perturbed system.

A. Potential scattering theory

Since resonant state expansions are connected with continuum processes (reactions and decays), it is natural to introduce resonance wave functions starting from scattering theory. We thus study the eigenfunctions related to the potential scattering of a spinless particle and if the potential is spherically symmetric, the equation to study is the radial Schrödinger equation

$$\begin{aligned}&(\mathcal{H}_\ell - k^2) u_\ell(k,r) \\ &= \Big(-\frac{d^2}{dr^2} + \frac{2m}{\hbar^2} V(r) + \frac{\ell(\ell+1)}{r^2} - k^2 \Big) u_\ell(k,r) = 0,\end{aligned} \tag{7}$$

where the wave number k is related to the energy by $k^2 = 2mE/\hbar^2$. The boundary condition that applies for the scattering solutions is

$$\psi_\ell(k,r) \to (-1)^\ell S_\ell(k) e^{ikr} - e^{-ikr} \ , \ r \to \infty, \tag{8}$$

and we will use the notation of Newton [12] to write

$$\psi_\ell(k,r) = \frac{k^{\ell+1}\varphi_\ell(k,r)}{f_\ell(-k)}, \tag{9}$$

where $\varphi_\ell(k,r)$ is the regular solution of (7) and $f_\ell(-k)$ is the Jost function [9]. We can also solve the radial Schrödinger equation for the resolvent (or complete Green's function)

$$(\mathcal{H}_\ell - k^2)\mathcal{G}_\ell(k;r,r') = -\delta(r-r'), \tag{10}$$

and if we apply the boundary condition that this should contain outgoing waves only, we can write

$$\mathcal{G}_\ell(k;r,r') = (-1)^{\ell+1} k^\ell \frac{\varphi_\ell(k,r_<) f_\ell(-k,r_>)}{f_\ell(-k)}, \tag{11}$$

where $f_\ell(-k,r')$ is the (outgoing) irregular solution of (7) and $r_<, r_>$ are, respectively, the lesser and greater of r and r'.

The resolvent $\mathcal{G}_\ell(k;r,r')$, the scattering function $\psi_\ell(k,r)$, and the partial wave S-matrix element $S_\ell(k)$ all have poles at the same places in the complex k plane, given by the zeros $k = k_n$ of the Jost function $f_\ell(-k) = 0$. Due to the symmetry $f_\ell(-k^*) = f_\ell^*(k)$, there are also poles at $k = \tilde{k}_n \equiv -k_n^*$. These zeros are naturally divided into four categories depending on their positions in the complex k plane, and we will sometimes use the letters $a-d$ to index them. We use the letter a to index the *antibound* (or virtual) states that are situated on the negative imaginary k axis ($k_a = -i\gamma_a$, $\gamma_a > 0$) and the letter b to index the *bound* states on the positive imaginary axis ($k_b = i\gamma_b$, $\gamma_b > 0$). Below the real axis and symmetrically with respect to the imaginary axis, we have pairs of resonance poles where we use the letter c for the *capturing* (or incoming) resonances ($\mathrm{Re}k_c < 0$) and the letter d for the *decaying* (or outgoing) resonances ($\mathrm{Re}k_d > 0$).

To each of these poles k_n we can define a corresponding eigenfunction in two ways. The first way is a generalization of the usual eigenvalue problem, i.e., to solve

$$(\mathcal{H}_\ell - {k_n}^2)u_n(r) = 0 \tag{12}$$

with purely outgoing boundary conditions

$$u_n(0) = 0\ ,\ u_n(r) \to e^{ik_n r},\ r \to \infty, \tag{13}$$

as suggested by Siegert [6]. These eigenfunctions are proportional to the regular solution, $u_n(r) = \varphi_\ell(k_n, r)/N_n$ and they actually form a *biorthogonal* set of functions, which means that they should be normalized using the overlap with the conjugate states $\tilde{u}_n$,

$$\langle \tilde{u}_m | u_n \rangle = \delta_{mn}, \tag{14}$$

where we have $\tilde{u}_n(r) = \varphi_\ell(k_n^*, r)/N_n^*$ and the properties of φ_ℓ imply $\tilde{u}_n(r) = u_n^*(r)$. For all of these states, except the bound states, the normalization integral

$${N_n}^2 = \int_0^\infty \varphi_\ell^2(k_n, r)\, dr \tag{15}$$

and the overlap integral $\int_0^\infty \varphi_\ell(k_m, r)\varphi_\ell(k_n, r)\, dr$ are at first sight divergent but we can, nevertheless, associate a certain number to each integral by the use of some regularization procedure (see Ref. [10] for a review and references). All of these regularization procedures give for the exponential integral

$$\int_R^\infty e^{iqr}\, dr = \frac{ie^{iqR}}{q},\ q \neq 0, \tag{16}$$

i.e., a natural analytic continuation of the convergent result. (The exponential with $q = 0$ is, of course, not regularizable in any sense.) This is all that we have to know about regularizations when considering a cutoff potential (1).

The alternative way of defining these eigenfunctions is to say that they should be given by the residues of the resolvent at its poles

$$\lim_{k \to k_n} (k^2 - {k_n}^2)\mathcal{G}_\ell(k; r, r') = u_n(r)u_n(r'). \tag{17}$$

This definition does not require any regularization procedure, and this makes it the natural one in Mittag-Leffler theory (Sec. II C). In both methods we can obtain an explicit expression for the normalization integral

$${N_n}^2 = \frac{f_\ell(k_n)\dot{f}_\ell(-k_n)}{4ik_n{}^{2\ell+2}}$$

(where the dot indicates derivation with respect to k), and this relation can be used to write down another important residue [11], namely,

$$\mathrm{Res}_{k=\pm k_n}\psi_\ell(k, r)\psi_\ell^*(k^*, r) = \pm\frac{i}{4}u_n(r)\tilde{u}_n^*(r'), \tag{18}$$

which is relevant for the development of the theory below.

We would here like to note that for the discrete states we have $\langle f|u_n\rangle\langle\tilde{u}_n|f\rangle = \langle\tilde{u}_n|f\rangle^2$ if f is a real function but there is no analog relation involving the scattering states $\psi_\ell(k, r)$. It is therefore sometimes convenient to define modified scattering functions

$$u_\ell(k, r) = \sqrt{\tfrac{2}{\pi}S_\ell^{-1}(k)}\psi_\ell(k, r) \tag{19}$$

and $\tilde{u}_\ell(k, r) = u_\ell^*(k, r)$ so that we can write

$$\frac{2}{\pi}\psi_\ell(k, r)\psi_\ell^*(k^*, r') = u_\ell(k, r)u_\ell(k, r')$$

and have $\frac{2}{\pi}\langle f|\psi_\ell(k)\rangle\langle\psi_\ell(k^*)|f\rangle = \langle\tilde{u}_\ell(k)|f\rangle^2$.

B. The completeness relation of Newton

Newton [12] proved that the set of bound states $u_b(r)$ together with the real scattering states $\psi_\ell(k, r)$ form a complete set

$$\delta(r - r') = \sum_b u_b(r)u_b(r') + \frac{1}{\pi}\int_{-\infty}^\infty dk\ \psi_\ell(k, r)\psi_\ell^*(k, r'), \tag{20}$$

which can be used to expand a function $h(r) = \int \delta(r - r')h(r')dr'$ as long as the function is square integrable. Using this completeness relation Newton also derived an expansion of the resolvent

$$\mathcal{G}_\ell(q; r, r') = \sum_b \frac{u_b(r)u_b(r')}{q^2 - {k_n}^2} + \frac{1}{\pi}\int_{-\infty}^\infty dk\ \frac{\psi_\ell(k, r)\psi_\ell^*(k, r')}{k(q - k)} \tag{21}$$

valid in the upper half plane (see also [11]).

C. Completeness relations in Mittag-Leffler theory

The Mittag-Leffler theorem deals with the convergence of a pole expansion of a meromorphic function [13]. Here we consider the poles of the resolvent corresponding to a cutoff potential (1). It is therefore natural to restrict oneself to a limited region of the radial space by introducing the projection operator P [14]

$$P\psi(r) = \begin{cases} \psi(r), & r \leq R_c \\ 0, & r > R_c \end{cases} \tag{22}$$

with $R_c < R_C$. This restriction is also necessary to prove the convergence [14] of

$$\langle\Phi_1|P\mathcal{G}_\ell(k)P|\Phi_2\rangle = \sum_n \frac{\langle\Phi_1|P|u_n\rangle\langle\tilde{u}_n|P|\Phi_2\rangle}{2k_n(k - k_n)}, \tag{23a}$$

which implies the validity of the resolvent expansion

$$\mathcal{G}_\ell(k; r, r') = \sum_n \frac{u_n(r)u_n(r')}{2k_n(k - k_n)}\ ,\ r, r' < R_C, \tag{23b}$$

where the functions u_n in the numerator are the same as in Eq. (17). Then using the findings [14] that

$$\lim_{k \to \infty} k^p\langle\Phi_1|P\mathcal{G}_\ell(k)P|\Phi_2\rangle = \delta_{p,2}\langle\Phi_1|P|\Phi_2\rangle \tag{24a}$$

when $p = 1, 2$, or [13]

$$\mathcal{G}_\ell(k; r, r') \to \frac{\delta(r - r')}{k^2} + O(k^{-3})\ ,\ k \to \infty \tag{24b}$$

one can derive the completeness relations

$$\sum_n \frac{\langle\Phi_1|P|u_n\rangle\langle\tilde{u}_n|P|\Phi_2\rangle}{2k_n} = 0, \tag{25a}$$

$$\frac{1}{2}\sum_n \langle\Phi_1|P|u_n\rangle\langle\tilde{u}_n|P|\Phi_2\rangle = \langle\Phi_1|P|\Phi_2\rangle \tag{25b}$$

and

$$\sum_n \frac{u_n(r)u_n(r')}{2k_n} = 0, \tag{25c}$$

$$\frac{1}{2}\sum_n u_n(r)u_n(r') = \delta(r-r')\ ,\ r,r' < R_C, \tag{25d}$$

respectively. The above expansions mean that we have

$$P|\hat{\Phi}_i\rangle \equiv \frac{1}{2}\sum_n P|u_n\rangle\langle\tilde{u}_n|P|\Phi_i\rangle \to P|\Phi_i\rangle, \tag{26}$$

but since the convergence is only *weak* [14], this does *not* imply that

$$\langle\hat{\Phi}_1|P|\hat{\Phi}_2\rangle \to \langle\Phi_1|P|\Phi_2\rangle,$$

which indicates that the Mittag-Leffler expansions sometimes are of more mathematical than practical interest. This we also expect from the fact that for the diverging functions, the value of the finite integral $\langle\tilde{u}_n|P|\Phi_i\rangle$ might have no similarity to the value of the regularized integral $\langle\tilde{u}_n|\Phi_i\rangle$.

In Ref. [13] the factor $\frac{1}{2}$ in Eqs. (25a)–(25d) was considered to indicate linear dependence among the u_n and the term "overcompleteness relation" was suggested for Eq. (25d). Since this linear dependence is only present in the limited radial range used in Mittag-Leffler theory, and not in the infinite range that we consider in this paper, we choose here to use other names for the relations above.

III. VARIOUS COMPLETENESS RELATIONS

In this section we derive a number of completeness relations in terms of scattering states and discrete states. The former states are defined by an integration contour C in the complex k plane (from $-\infty$ to $+\infty$) that approach the real axis as $|k| \to \infty$ and the latter by the poles of the resolvent (zeros of the Jost function) that are enclosed by this contour and an infinite semicircle in the upper half plane. It is sometimes convenient to divide this contour into two conjugate parts, $C = C^+ + C^-$, e.g., such that k is on $C^\pm$ if $\pm\mathrm{Re}k > 0$. In Figs. 1–3 we show the different contours used in this paper and the distributions of zeros of the relevant Jost functions. We will here only consider contours that are either *inversion symmetric* (such as R, L, Z), i.e., if k is on C then so is $-k$, or *reflection symmetric* (such as R, W, U), i.e., if k is on C then so is $-k^*$ (see Fig. 1). If we define the complex conjugate contour C^* (also oriented from $-\infty$ to $+\infty$) by all k^*, where k is on C, we can from the reflection symmetric contours form inversion symmetric contours such as $\Omega = W^* - R + W$ and $\Upsilon = U^* - R + U$ (see Fig. 2).

The proof of completeness is made using the theory of analytic functions with the analytic properties of the resolvent and scattering functions governed essentially by the Jost function. We choose in this section to write the completeness relations as unit operators (resolutions of unity or projection operators) in order to show how the basis states of different completeness relations are related through the analytic properties of the integrand of the integrals used in their derivation. We thus first concentrate on the derivation and defer to later the discussions of validity.

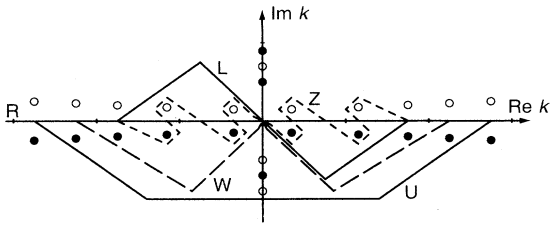

FIG. 1. Contours in the complex k plane used to define the continuum of various completeness relations. The dots mark the positions of the zeros of the Jost function $f_\ell(-k)$ [i.e., the poles of the resolvent $\mathcal{G}_\ell(k;r,r')$] and the rings mark the positions of the zeros of $f_\ell(k)$.

A. Newton-Berggren derivation of completeness

The proof of completeness as given by Newton [12] was modified by Berggren [4] for the inclusion of a finite number of resonances and a complex continuum. In this proof we consider the integral $I_\Gamma = \int_\Gamma dk\, k\mathcal{G}_\ell(k)$, where $\Gamma = S + C$ is a contour in the complex k plane that consists of two parts, one infinite semicircle in the upper half plane S and one contour C of the type discussed above. We evaluate the integral I_Γ by Cauchys theorem, the integral I_S is evaluated explicitly and the remaining contour integral, I_C, can be rewritten in terms of scattering functions if (and only if) the contour is inversion symmetric. In this case we obtain the proper *completeness relation*

$$\mathbb{1} = \sum_{k_n\in\mathbf{C}} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_C |\psi_\ell(k)\rangle\, dk\, \langle\psi_\ell(k^*)|, \tag{27}$$

where $\mathbf{C}$ is the domain in the k plane above the C con-

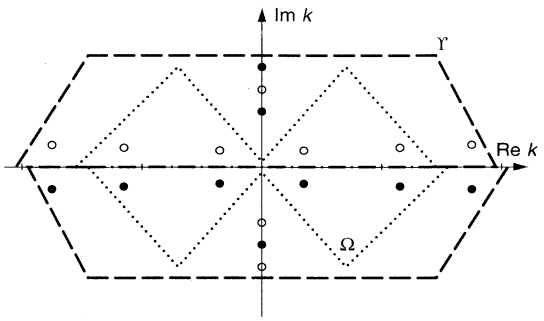

FIG. 2. Inversion symmetric contours in the complex k plane created from the reflection symmetric contours in Fig. 1, $\Omega = W^* - R + W$ and $\Upsilon = U^* - R + U$.

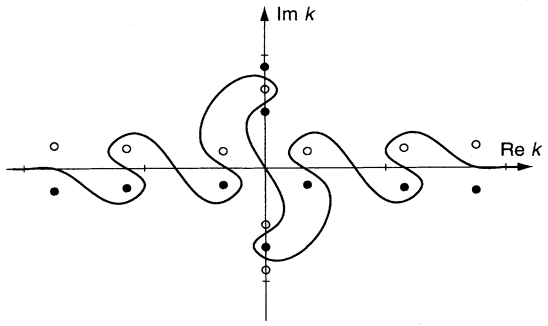

FIG. 3. Contour in the complex k plane that define the continuum in the proper completeness relation $\mathbb{1} = \sum_{abcd} |n\rangle\langle\tilde{n}| + \frac{1}{\pi}\int_C |k\rangle dk\langle k^*|$ where all kinds of pole states are included in the discrete part.

tour. We primarily think of C as being either R, L, or Z, and in these cases we can rewrite the discrete part of (27)

$$\sum_{k_n\in\mathbf{R}} = \sum_{n=b}, \quad \sum_{k_n\in\mathbf{L}} = \sum_{n=b,d}, \quad \sum_{k_n\in\mathbf{Z}} = \sum_{n=b,c,d}$$

to show explicitly what kinds of discrete states that are included in the complete set. Above we noted that also Ω and Υ are inversion symmetric and can be used to derive completeness relations like (27), where we now have to interpret $\mathbf{C}$ as the sum of $\mathbf{C}^*$, i.e., the domain in k plane above the C^* contour, and $\mathbf{C}\backslash\mathbf{R}$, the domain between the C and the R contours. We can here write

$$\sum_{k_n\in\Omega} = \sum_{n=b,c,d}, \quad \sum_{k_n\in\Upsilon} = \sum_{n=a,c,d},$$

thus indicating the fact that the contours Z and Ω actually are equivalent. The necessity of using inversion symmetric contours in the derivation of completeness means that, due to the symmetry of the integrand of the continuum part of (27), we only need one of the conjugate halves of the contour, since $\int_{C^-} |k\rangle dk\langle k^*| = \int_{C^+} |k\rangle dk\langle k^*|$. This is convenient if we wish to formulate completeness using energy as the variable of integration instead of wave number and, of course, if we need to perform a numerical integration. We cannot include *both* the bound states and the antibound states in the discrete part of a proper completeness relation when using the inversion symmetric contours above. Instead we combine the above Z contour with a part of the contour suggested in [15] so as to form the contour of Fig. 3. We then include *all* kinds of pole states in the discrete part

$$\sum_{k_n\in\mathbf{C}} = \sum_{n=a,b,c,d}$$

at the expense of having an extremely complicated contour that seems to have little physical meaning and certainly cannot be neglected, since it contains hidden contributions from all the poles. Even if this is a perfectly valid completeness relation, it does not help us to understand the structure of the important final relations below so we will only exceptionally consider this contour.

In Sec. IV C we apply the definition of the resolvent (10) to a proper spectral resolution and obtain the operator

$$\mathbf{0} = \frac{1}{\pi}\int_C \frac{|\psi_\ell(k)\rangle\, dk\, \langle\psi_\ell(k^*)|}{k}, \tag{28}$$

which we interpret as a zero operator. The reason is that there is an extra factor in the integrand of (28) that breaks the inversion symmetry of the integrand of (27) so that now $\int_{C^-} |k\rangle \frac{dk}{k} \langle k^*| = -\int_{C^+} |k\rangle \frac{dk}{k} \langle k^*|$ and thus $\int_C |k\rangle \frac{dk}{k}\langle k^*| = 0$. We will anyway, throughout this paper, continue to treat (28) analytically in the same way as (27). Since (28) at first sight seems to imply a linear dependence among the eigenstates, we find it appropriate to call (28), and the relations that we will derive from it, *overcompleteness relations.*

B. Derivation using analytic continuation

Here we present a straightforward method of deriving completeness relations by starting from the relation of Newton

$$\mathbb{1} = \sum_{n=b} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_R |\psi_\ell(k)\rangle\, dk\, \langle\psi_\ell(k^*)| \tag{29}$$

written in such a way that the integrand is a meromorphic function of k with poles given by $f_\ell(-k) = 0$ and $f_\ell^*(-k^*) = f_\ell(k) = 0$. The residues of the product of scattering functions in the integrand at these poles are given by (18). We can thus, by deforming the contour continuously and using Cauchy's theorem, extract the contributions from the resonant states that are hidden in the continuum integral and write them in the same form as the bound state contributions. It has often (more or less well justified) been assumed that by this the remaining continuum contribution only would be a smooth background, hopefully negligible, or even vanishing. This of course depends on the shape of the contour but not necessarily on the number of states explicitly included in the discrete part which will be illustrated below.

If we deform the real axis R into the L contour we get, using $\int_{L-R} = \sum_d$, the old Berggren completeness relation [4]

$$\mathbb{1} = \sum_{n=b,d} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_L |\psi_\ell(k)\rangle\, dk\, \langle\psi_\ell(k^*)|. \tag{30}$$

Since the resonance functions are complex, the discrete contribution from this relation to the expansion of a real quantity is also complex and the continuum term contains the restoring imaginary part. The real part of the discrete contribution might, however, be a good approximation in this case, and this has led to various "rules" for interpretation of such expansions and matrix elements involving resonant states [4, 16, 17].

If we instead had deformed the real axis into the Z contour, $\int_{Z-R} = \sum_{c,d}$, we would have obtained the relation suggested by Berggren [18],

$$\mathbb{1} = \sum_{n=b,c,d} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_Z |\psi_\ell(k)\rangle\, dk\, \langle\psi_\ell(k^*)| \quad (31)$$

to transfer the restoring imaginary part from the continuum to the discrete part. Unfortunately the discrete part is no longer a good approximation due to the doubling of the resonance contribution and the continuum is now needed to compensate for this.

The relations (30) and (31), with the continuum integrals, were also derived in Sec. III A and are proper completeness relations but with different ranges of validity as discussed below.

In this method there seems to be no restriction to inversion symmetric contours so that if we deform the real axis into the W contour, $\int_{W-R} = \frac{1}{2}\sum_{c,d}$, we get

$$\mathbb{1} = \sum_{n=b} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{2}\sum_{n=c,d} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_W |\psi_\ell(k)\rangle dk\, \langle\psi_\ell(k^*)|. \quad (32)$$

The discrete part of this relation will give a real contribution to the expansion of a real quantity, just as the discrete part of (31) will, but compared to that it contains a factor $\frac{1}{2}$ to compensate for the double counting of the resonance contribution so it might be just as good an approximation as the discrete part of (30) but without the need of a special treatment of false imaginary parts. The relation (32) can also be derived using the inversion symmetric contour Ω if we split the integral into two parts, $\int_\Omega = \int_{W^*-R} + \int_W$, and evaluate the closed integral $\int_{W^*-R}$ using Cauchy and the residues (18), $\int_{W^*-R} = -\frac{1}{2}\sum_{c,d}$.

If we continue deforming the W contour into the U contour, $\int_{U-W} = \frac{1}{2}(\sum_a - \sum_b)$, or taking (27) with $C = \Upsilon$ and evaluating $\int_{U^*-R} = -\frac{1}{2}(\sum_{a,c,d} - \sum_b)$, we get as suggested by Romo [19]

$$\mathbb{1} = \frac{1}{2}\sum_{n=a,b,c,d} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_U |\psi_\ell(k)\rangle dk\, \langle\psi_\ell(k^*)|. \quad (33)$$

The discrete part of this relation is the same as in Mittag-Leffler theory and the factor $\frac{1}{2}$ indicates, comparing with (32), that the bound states and antibound states might give similar contributions but the need for both of them also indicates that the eventual difference between them is formally important and thus not compensated for by the remaining U integral.

To every completeness relation in this subsection there is a corresponding overcompleteness relation obtained by deforming the contour in (28), from $C = R$ to $C = L$, Z, W, or U, now making use of the residues

$$\mathrm{Res}_{k=\pm k_n} \frac{\psi_\ell(k,r)\psi_\ell^*(k^*,r)}{k} = \frac{i}{4}\frac{u_n(r)\tilde{u}_n^*(r')}{k_n} \quad (34)$$

or equivalently taking (28) with the same evaluation of closed integrals as made above. We noted above that this relation is identically zero when the contour is inversion symmetric and the contributions from the residues (34) are cancelling when deforming to another inversion symmetric contour. But when we deform C into a reflection symmetric contour, the symmetry of the integrand is no longer such that it makes the integral vanish and the contributions from the residues are no longer cancelling. We thus obtain the more interesting relation

$$\mathbf{0} = \frac{1}{2}\sum_{n=a,b,c,d} \frac{|u_n\rangle\langle\tilde{u}_n|}{k_n} + \frac{1}{\pi}\int_U \frac{|\psi_\ell(k)\rangle\, dk\, \langle\psi_\ell(k^*)|}{k}. \quad (35)$$

In fact, we see in the numerical studies below that this overcompleteness relation sometimes is as important as the corresponding reduced completeness relation (33). These two relations are very interesting, since the discrete parts of them look the same as in Mittag-Leffler theory (Sec. II C). We consider the analytic continuations made here to be the link between the eigenfunction theory and the Mittag-Leffler theory.

C. Validity of completeness relations

The completeness relation of Newton, (20) or (29), with bound states and real continuum states is valid for expanding a function

$$\Phi(r) = \sum_b u_b(r)\langle u_b|\Phi\rangle + \frac{1}{\pi}\int_R dk\ \psi_\ell(k,r)\langle\psi_\ell(k^*)|\Phi\rangle, \quad (36)$$

provided the function is square integrable. This class of functions includes those with exponential asymptotics, $\Phi(r) \to e^{iqr}$, $r \to \infty$, with $\mathrm{Im}q > 0$, i.e., with q above the R contour ($q \in \mathbf{R}$). In Ref. [4] Berggren states that the relation (30) could be used for expanding functions with exponential asymptotics and q above the L contour ($q \in \mathbf{L}$). This condition was based on the regularization procedure used to calculate overlaps with the complex continuum states on the L contour. Although we now believe that we can assign a unique number to every overlap between two functions with exponential asymptotics, we stick to the condition above. The main reason for this is that we cannot project the capturing resonances onto the space spanned by the bound states and decaying resonances in (30), since $\langle\tilde{u}_n|u_c\rangle = 0$, $n = b, d$ and $\langle\psi_\ell(k^*)|u_c\rangle = 0$. For the completeness relation (31) the corresponding condition would be $q \in \mathbf{Z}$. We can now generally say that the completeness relation (27) is valid for expanding a function

$$\Phi(r) = \sum_{k_n\in\mathbf{C}} u_n(r)\langle\tilde{u}_n|\Phi\rangle + \frac{1}{\pi}\int_C dk\ \psi_\ell(k,r)\langle\psi_\ell(k^*)|\Phi\rangle \quad (37)$$

with exponential asymptotics, $\Phi(r) \to e^{iqr}$, $r \to \infty$, where $q \in \mathbf{C}$. For the cases $C = \Omega$ and $C = \Upsilon$ this might not be obvious but can be understood from the following considerations.

That there is a special interest (also from an analytic

point of view) in studying functions with exponential asymptotics is understood if we look at (36) and deform the contour. We then have to consider the poles given by $|\psi_\ell(k)\rangle\langle\psi_\ell(k^*)|$ (as in Sec. III B) but also the possibility of an extra singularity in $\langle\psi_\ell(k^*)|\Phi\rangle$ that is not due to a zero of the Jost function. To see this singularity explicitly, we take an S-wave scattering function of a cutoff potential (1) so that $\psi_0(k,r) = S_0(k)e^{ikr} - e^{-ikr}$, $r > R_C$. If then $\Phi(r) = e^{iqr}$, $r > R_C$, we have in $\langle\psi_0(k^*)|\Phi\rangle$ the integral

$$\int_{R_C}^{\infty} \left(S_0(k^*)e^{ik^*r} - e^{-ik^*r}\right)^* e^{iqr}\, dr$$

$$= S_0^*(k^*)\int_{R_C}^{\infty} e^{-i(k-q)r}\, dr - \int_{R_C}^{\infty} e^{i(k+q)r}\, dr$$

$$= S_0^{-1}(k)\frac{e^{-i(k-q)R_C}}{i(k-q)} + \frac{e^{i(k+q)R_C}}{i(k+q)}, \tag{38}$$

where we see that we have two extra singularities at $k = \mp q$ to consider when we deform the contour in (36). In the proof of completeness we only use the overlap with a purely outgoing function and thus we need only to treat one extra singularity at $k = -q$. This pole is not enclosed by the contour $\Gamma = S + C$ as long as $q \in \mathbf{C}$, which supports the criterium for validity of the completeness relations (27) with C inversion symmetric suggested above. In the method of Sec. III B, however, both the singularities at $k = \mp q$ might be encountered when deforming R into C. But these two singularities give cancelling contributions, again a manifestation of the importance of using an inversion symmetric contour. If we deform R into a reflection symmetric contour like U, we will only encounter one singularity, viz., the one at $k = -q$ if $\mathrm{Im}q > 0$. To obtain a correct treatment of this extra pole when deforming to the U contour, we must, however, not start from the R contour but rather from the contour in the completeness relation, which is valid for the function we are expanding, i.e., we must choose the inversion symmetric contour C in (27) so that $q \in \mathbf{C}$. When we deform *this* contour into the U contour, we will encounter the singularity $k = -q$ (at least sooner or later if the U contour can be extended without limitations). The expansion of $|\Phi\rangle$ using (33) would then have to be complemented by a closed contour integral around $k = -q$ (denoted by $-\oint_{k=-q}$ if the orientation is positive) and, if the singularity is of first order, this would be proportional to $|\psi_\ell(-q)\rangle$, which has rather absurd consequences. As will be seen in the next section, the expansion with such a complementary integral can only be used under certain conditions to calculate overlaps with functions, which have exponential asymptotics.

Thus in the unit operator (27), with C inversion symmetric, both the discrete part and the continuum part are idempotent (in addition to $\mathbb{1}^2 = \mathbb{1}$) so the relations (29), (30), and (31) are certainly proper completeness relations. This is not the case for the relations (32) and (33), where the discrete part and the continuum part (although still orthogonal) are not idempotent. This holds despite the fact that they are derived from the idempotent operators (27) with $C = \Omega$ and Υ. When we derive (33) from (27), with $C = \Upsilon$, we split the continuum part $\int_\Upsilon$ into two parts $\int_U$ and $\int_{U^*-R}$, neither of which is idempotent, but, since they are not orthogonal $[\langle(-k)^*|k\rangle \neq 0]$, the total unit operator is idempotent. The critical point is that we reduce the closed continuum $\int_{U^*-R}$ into a sum $\frac{1}{2}(\sum_b - \sum_{acd})$, but, even if this sum is equivalent to the closed integral, it is orthogonal to $\int_U$, which makes the unit operator (33) nonidempotent. Even if (32) and (33) are not projection operators, it was suggested in [11] to call them *reduced completeness relations*, since they might still provide us with valid resonant state expansions.

IV. RESONANT STATE EXPANSIONS

By a resonant state expansion (RSE) we do not mean just a pole expansion but a way of expressing a quantity as a sum where each term is associated with one specific state u_n (or equivalent to a specific pole, k_n, of the resolvent) with the possible addition of a smooth and small continuum part. This can be achieved by using a completeness relation or an expansion of the resolvent (if the matrix element to be expanded involves the resolvent). In this paper we consider only the former possibility in detail, since it is more general and the analytic considerations involved are the same in both cases. From Mittag-Leffler theory we expect that the best discrete approximation is obtained if all kinds of pole states are included so that the reduced completeness relation (33) would seem preferable to use. For a proper treatment of eventual extra singularities we choose, as suggested in Sec. III C, to start from a valid completeness relation (27) and then deform the inversion symmetric contour C into the U contour, taking into account the full analytic structure of the integrand obtained. The difference from a straightforward use of the relation (33) is due to the uncontrolled interchange of integration orders made in the derivation and this will show up if the asymptotic behavior of the functions in the matrix element to be expanded is of a certain kind.

A. RSE of matrix element

Here we study the expansion of a matrix element (or overlap) obtained by the use of a resolution of unity in terms of eigenstates $\langle\tilde{\Phi}_1|\Phi_2\rangle = \langle\tilde{\Phi}_1|\mathbb{1}|\Phi_2\rangle$. The sum rule studies by Berggren [20] and Romo [21] of $\langle\tilde{\Phi}_1|AB|\Phi_2\rangle = \langle\tilde{\Phi}_1|A\mathbb{1}B|\Phi_2\rangle$ can be included by associating $(A\Phi_1)(r)$ and $(B\Phi_2)(r)$ with one of the classes of functions below and will thus not be explicitly considered here. The expansion of a matrix element using the proper completeness relation (27), i.e.,

$$\langle\tilde{\Phi}_1|\Phi_2\rangle = \sum_{n\in\mathbf{C}}\langle\tilde{\Phi}_1|u_n\rangle\langle\tilde{u}_n|\Phi_2\rangle + \frac{1}{\pi}\int_C \langle\tilde{\Phi}_1|\psi_\ell(k)\rangle\, dk\, \langle\psi_\ell(k^*)|\Phi_2\rangle, \tag{39}$$

is used as a starting point for derivations of expansions in terms of discrete states and complex scattering states by

deforming the inversion symmetric contour C into the U contour. We will then pass over some of the poles of the integrand $\langle\tilde{\Phi}_1|\psi_\ell(k)\rangle\langle\psi_\ell(k^*)|\Phi_2\rangle$ and the contributions from those corresponding to the zeros of the Jost function is evaluated using the residues (18). But as we saw in Sec. III C, there might also be extra poles if the functions $\Phi_i(r)$ have exponential asymptotics. We therefore find it convenient to consider basis states from a cutoff potential (1) and to define three classes of functions with different asymptotics: E functions, $\phi(r)$, with exponential asymptotics $\phi(r) \to e^{iqr}$, $r \to \infty$; F functions, $h(r)$, that decay faster than exponentially, $e^{\zeta r}h(r) \to 0$, $r \to \infty$, $\forall\zeta$, and are not truncated within the range of the potential, i.e., there is $r > R_C$ so that $h(r) \neq 0$; and T functions, $\chi(r)$, that are truncated within the range of the potential $\chi(r) = 0$, $r > R_c$, $R_c < R_C$. Functions in this class can be created with the projection operator (22), $\chi = P\Phi$. We only consider functions that are sufficiently continuous in order not to fill the text with mathematical conditions. (For a more serious treatment of the class T one can consult [14].)

The class of truncated functions T is the easiest one to treat, since we can make use of results from Mittag-Leffler theory (Sec. II C)

$$\langle\tilde{\chi}_1|\chi_2\rangle = \frac{1}{2}\sum_{n=a,b,c,d}\langle\tilde{\chi}_1|u_n\rangle\langle\tilde{u}_n|\chi_2\rangle, \tag{40}$$

$$0 = \sum_{n=a,b,c,d}\frac{\langle\tilde{\chi}_1|u_n\rangle\langle\tilde{u}_n|\chi_2\rangle}{2k_n}, \tag{41}$$

which means that the U integrals in (33) and (35) are exactly vanishing in this case.

For the classes of functions that are not truncated, we generally expect the U integral in (33) to be nonvanishing. We saw in Sec. III C that functions with exponential asymptotics will give rise to extra poles in the integrand and for the matrix element $\langle\tilde{\phi}_1|\phi_2\rangle$ they are seen from the integrand $\langle\tilde{\phi}_1|k\rangle\langle k^*|\phi_2\rangle$ to be localized at $k = \mp q_2$ and $k = \mp q_1$. We find numerically that the remaining U integral in this case actually vanishes, thus leaving us with the expansion

$$\langle\tilde{\phi}_1|\phi_2\rangle = \frac{1}{2}\sum_{n=a,b,c,d}\langle\tilde{\phi}_1|u_n\rangle\langle\tilde{u}_n|\phi_2\rangle - \frac{1}{\pi}\Big(\oint_{k=-q_2} + \oint_{k=-q_1}\Big)\langle\tilde{\phi}_1|\psi_\ell(k)\rangle\, dk\, \langle\psi_\ell(k^*)|\phi_2\rangle. \tag{42}$$

If these poles are of first order, it is possible to express the closed integrals as residues in terms of scattering functions with the complex momenta $-q_2$ and $-q_1$. Obviously we would have missed these extra terms in (42) if we had made straightforward use of (33) (and found the U integral vanishing). Due to the existence of an overcompleteness relation in the expansion of the overlap of class T functions (41) and the vanishing U integral in the class E overlap, it is interesting to speculate about having also

$$0 = \sum_{n=a,b,c,d}\frac{\langle\tilde{\phi}_1|u_n\rangle\langle\tilde{u}_n|\phi_2\rangle}{2k_n} - \frac{1}{\pi}\Big(\oint_{k=-q_2} + \oint_{k=-q_1}\Big)\langle\tilde{\phi}_1|\psi_\ell(k)\rangle\,\frac{dk}{k}\,\langle\psi_\ell(k^*)|\phi_2\rangle. \tag{43}$$

This is verified numerically simultaneous with (42).

So far we have mostly considered the U contour, since it is more challenging to understand how to use all the different kinds of basis states u_n and whether it is possible to obtain discrete expansions without too heavy restrictions on what they can expand. An expansion such as (39) is safe but one can, in general, not expect the C integral to be negligible. Since these unit operators are idempotent, we also have $\langle\tilde{\Phi}_1|\Phi_2\rangle = \langle\tilde{\Phi}_1|\mathbb{1}^2|\Phi_2\rangle$, which means that we could have formed expansions of the functions $|\Phi_i\rangle = \mathbb{1}|\Phi_i\rangle$ and then the expansion of the overlap from these expanded functions. The expansion of a function using a reflection symmetric contour deserves a subsection for itself.

B. RSE of functions

We will again concentrate on the U contour expansions, and, since we have already noticed that the resolution of unity (33) is not idempotent, we cannot use two expanded functions

$$|\Phi_i\rangle = \frac{1}{2}\sum_{n=a,b,c,d}|u_n\rangle\langle\tilde{u}_n|\Phi_i\rangle + \int_U|\psi_\ell(k)\rangle\, dk\,\langle\psi_\ell(k^*)|\Phi_i\rangle \tag{44}$$

to form the expansion of the overlap $\langle\tilde{\Phi}_1|\Phi_2\rangle$. But if at most one of the functions, $\Phi_2(r)$ say, has exponential asymptotics [and this function is expanded as in (44) with the addition of $\oint_{k=-q_2}$ if U has passed $-q_2$], we can use (44) to form the overlap [if the other function, $\Phi_1(r)$, is not expanded], since we have then only obtained $\langle\tilde{\Phi}_1|\mathbb{1}|\Phi_2\rangle$ as above. If the remaining U contour has not passed the pole $k = -q_2$, it is of course irrelevant which of the functions we expand, but if it has, we have, if the extra pole is of first order,

$$\oint_{k=-q_2}\psi_\ell(k,r)\,\frac{dk}{k}\,\langle\psi_\ell(k^*)|\phi_2\rangle = \frac{1}{-q_2}\oint_{k=-q_2}\psi_\ell(k,r)\,dk\,\langle\psi_\ell(k^*)|\phi_2\rangle. \tag{45}$$

If we in this case act on $|\phi_2\rangle$ with the sum of the "unit operator" (33) and q_2 times the "zero operator" (35), the singular integral contributions cancel out and we get

a purely discrete expansion

$$|\phi_2\rangle = \sum_{n=a,b,c,d} |u_n\rangle \frac{k_n + q_2}{2k_n} \langle \tilde{u}_n | \phi_2 \rangle, \tag{46}$$

which is valid even if ϕ_2 is one of the u_n. This expansion can be used to give a purely discrete expansion of $\langle \tilde{\chi}_1 | \phi_2 \rangle$. Even if the set of functions u_n is in some sense overcomplete, or rather that its completeness is reduced, it seems that we can to some extent compensate for this by making simultaneous use of both the reduced completeness relation (33) and the overcompleteness relation (35).

C. RSE of resolvent

The resonant state expansion of the resolvent $\mathcal{G}_\ell(q; r, r')$ has recently been thoroughly studied in [11] so we just comment on it here. Again we can use the method of Sec. III B, i.e., starting from the expansion of Newton (21), valid for $q \in \mathbf{R}$, and then deforming the real axis into C and making use of the residues (18) whenever a pole of the integrand is passed over. Alternatively one could start from the proper completeness relation (27) and use this, as Newton did, to derive the expansion

$$\mathcal{G}_\ell(q; r, r') = \sum_{k_n \in \mathbf{C}} \frac{u_n(r) \tilde{u}_n^*(r')}{q^2 - {k_n}^2} + \frac{1}{\pi} \int_C dk \, \frac{\psi_\ell(k, r) \psi_\ell^*(k^*, r')}{k(q-k)}. \tag{47}$$

If we use this expansion in the definition of the resolvent (10) we get

$$\begin{aligned} \mathbb{1} &= (q^2 - \mathcal{H}_\ell)\mathcal{G}_\ell(q) \\ &= \sum_{k_n \in \mathbf{C}} |u_n\rangle \frac{q^2 - {k_n}^2}{q^2 - {k_n}^2} \langle \tilde{u}_n| + \frac{1}{\pi} \int_C dk \, |\psi_\ell(k)\rangle \frac{q^2 - k^2}{k(q-k)} \langle \psi_\ell(k^*)| \\ &= \sum_{k_n \in \mathbf{C}} |u_n\rangle \langle \tilde{u}_n l| + \frac{1}{\pi} \int_C dk \, |\psi_\ell(k)\rangle \frac{k+q}{k} \langle \psi_\ell(k^*)|. \end{aligned} \tag{48}$$

In the last line here, we recognize the completeness relation (27) and the rest we interpret as q times the proper zero operator (28).

For a more thorough treatment of the analyticity one can instead consider the expansion of the double integral $\langle \Phi_1 | \mathcal{G}_\ell(k) | \Phi_2 \rangle$ and thereby obtain the same modifications as in Sec. IV A. The expansion of the single particle response function, $R_\ell(k) = \langle f | \mathcal{G}_\ell(k) | f \rangle$, was studied numerically in [22] and was commented on in [11] as will be done below. One of the major insights of [11] was the importance of the symmetry of the quantity to be expanded. For a proper completeness relation this is the inversion symmetry of the integrand of (20), while for the resolvent expansion it is important to use a reflection symmetric contour, since $\mathcal{G}_\ell(-k^*) = \mathcal{G}_\ell^*(k)$. Again it was found that the U contour gave the most complete treatment of the pole structure of the resolvent

$$\mathcal{G}_\ell(q; r, r') = \sum_{n=a,b,c,d} \frac{u_n(r) \tilde{u}_n^*(r')}{2k_n(q - k_n)} + \frac{1}{\pi} \int_U dk \, \frac{\psi_\ell(k, r) \psi_\ell^*(k^*, r')}{k(q-k)}. \tag{49}$$

The discrete part is recognized from the Mittag-Leffler expansion (23b) so we conclude that the U integral in the expansion of $\langle \chi | \mathcal{G}_\ell(k) | \chi \rangle$ is vanishing. For response functions involving other types of form factors f, the conclusions of the previous subsections should be applicable.

We would here also like to note that if we use the expansion (49) in the definition of the resolvent

$$\begin{aligned} \mathbb{1} &= (q^2 - \mathcal{H}_\ell)\mathcal{G}_\ell(q) \\ &= \sum_{n=a,b,c,d} |u_n\rangle \frac{k_n + q}{2k_n} \langle \tilde{u}_n| \\ &\quad + \frac{1}{\pi} \int_U dk \, |\psi_\ell(k)\rangle \frac{k+q}{k} \langle \psi_\ell(k^*)| = \text{“}\mathbb{1} + q\mathbf{O}\text{”} \end{aligned} \tag{50}$$

we get in the final right-hand side the sum of the “unit operator” (33) and q times the “zero operator” (35). The discrete part of this sum was also found in [23] in the framework of Mittag-Leffler theory, but there only used to state that the discrete parts of (33) and (35) must be valid separately. What we found here though indicates that both these relations need, under certain conditions, to be used *together* for a complete treatment in terms of discrete states over the infinite radial region. Since we seem to have a q-dependent unit operator, the validity is of course not general but it can, as we saw above, give rise to efficient expansions and it will make possible the interpretation of the solutions to a certain matrix equation (see Sec. V B).

D. Numerical illustrations

1. *Expanisons of matrix element*

We will first illustrate the proper completeness relation (27), the reduced completeness relation (33), and the overcompleteness relation (35) by expanding the matrix element $\langle \Phi_1 | \Phi_2 \rangle$ where we take $\Phi_1 = \Phi_2 = f$ and the

(class F) function f is chosen to be real and of Gaussian form

$$f(r) = \exp\left[-\left(\frac{r-6.75}{0.75}\right)^2\right]. \tag{51}$$

As the basis $\{|n\rangle\}$ we choose the $\ell = 0$ states of the $V_\square = 23$ MeV and $R_\square = 7$ fm square well (see Table I) which means that the integral $\langle f|f\rangle$ gets a significant contribution from the radial region outside the cutoff radius of the potential $R_C = R_\square$. Thus the Mittag-Leffler expansions are not applicible and the continuum integral in the expansions derived above is expected to be important.

In Fig. 4(a) we show as function of the number of included states, $\sum(N) = \sum_n^N$, the discrete part of the expansions

$$\langle f|f\rangle = \sum_{n=b} \langle u_n|f\rangle^2 + \int_{R^+} \langle \tilde{u}_\ell(k)|f\rangle^2\, dk, \tag{52a}$$

$$\langle f|f\rangle = \sum_{n=b,d} \langle \tilde{u}_n|f\rangle^2 + \int_{L^+} \langle \tilde{u}_\ell(k)|f\rangle^2\, dk, \tag{52b}$$

$$\langle f|f\rangle = \frac{1}{2}\sum_{n=a,b,c,d} \langle \tilde{u}_n|f\rangle^2 + \int_{U^+} \langle \tilde{u}_\ell(k)|f\rangle^2\, dk, \tag{52c}$$

$$0 = \sum_{n=a,b,c,d} \frac{\langle \tilde{u}_n|f\rangle^2}{2k_n} + \int_{U^+} \frac{\langle \tilde{u}_\ell(k)|f\rangle^2}{k}\, dk. \tag{52d}$$

[It is possible to simplify the integral

$$\frac{1}{\pi}\int_U \langle \Phi_1|\psi_\ell(k)\rangle\, dk\, \langle \psi_\ell(k^*)|\Phi_2\rangle$$

to $\int_{U^+}\langle \tilde{u}_\ell(k)|f\rangle^2\, dk$ only if $\Phi_1 = \Phi_2 = f =$ real.] Since the Mittag-Leffler conditions are not fulfilled, the discrete parts do not converge as $N \to \infty$. Therefore we illustrate also the continuum part of the expansions.

We approximated the complex contours L^+ and U^+ by straight lines and parametrized them in the k plane as

$$L^+ : 0 + 0i \to 2 - 1.1i \to \infty - 1.1i,$$
$$U^+ : 0 - 1.1i \to \infty - 1.1i,$$

but we calculated them only up to a finite k value, $k_{\max}$, which correspond to an energy $E_{\max}$. In Fig. 4(b) we show as a function of $E = \mathrm{Re}E_{\max}$ the continuum contribution to the expansions, $\int(E) = \sum_n + \int_0^{k_{\max}}$, which start at the values of the limits of $\sum(N)$ seen in Fig. 4(a). The real part of the energy of the last included states in Fig. 4(a) is chosen consistent with the energy interval in Fig. 4(b). We see that it is here sufficient to include states with energies up to 400 MeV to obtain satisfactory expansions. The question of how the contours approach the real axis as $k \to \infty$ and the selection of asymptotic resonances is found to be unimportant.

The main purpose of this example was to show that the analytically continued expansions work and can be conveniently performed numerically.

2. *Expanisons of overlaps*

The importance of the continuum in the form of the singular integrals in (42) and (43) is illustrated by taking ϕ_i as the $\ell = 0$ eigenstates of the $V_\square = 28$ MeV and $R_\square = 7$ fm square well and the basis states from the $V_\square = 23$ MeV well (see Table I for both). We give in Table II the values of the integrals $-\frac{1}{\pi}\oint_{k=-q_i}\langle\tilde{\phi}_1|k\rangle dk\langle k^*|\phi_2\rangle$, $i = 1, 2$, which can be calculated as simple residues except when $q_1 = q_2$ and we have a double pole. Even if we include only the basis states listed in Table I, we reproduce the value $\langle\tilde{\phi}_i|\phi_j\rangle = \delta_{ij}$ with an accuracy of 0.0005 and the zero of Eq. (43) within 0.0002. The contribution from the integrals is such that keeping only the discrete parts in the expansions (42) and (43) would be a poor approximation in most cases.

Note that we have no problem with defining and calculating the overlap between a bound state and an antibound state, since we can start from the completeness relation corresponding to the contour in Fig. 3. Compare with the discussion in Ref. [15] where both bound states and antibound states were used in an attempt to expand the unit operator.

3. *Expansion of functions*

We illustrate the discussions above by showing in Fig. 5 the convergence of several expansions of the matrix element $\langle\psi_\mu|f^2|\psi_\nu\rangle$, where we take $\psi_\mu = \psi_\nu$ to be the third $\ell = 0$ bound state of the $V_\square = 28$ MeV and $R_\square = 7$ fm square well (see Table I). For the form factor we take $f(r) \propto r(R_\square - r)P(r)$, where P is defined in (22) with $R_c = R_\square$, normalized so that $\langle f|f\rangle = 1$. In Fig. 5(a) we show the expansions $\frac{1}{2}\sum_n\langle\tilde{n}|f\rangle^2 \to 1$ and $\sum_n \frac{\langle\tilde{n}|f\rangle^2}{2k_n} \to 0$. As basis, $\{|n\rangle\}$, we use the states

TABLE I. The lowest eigenvalues of the $\ell = 0$ basis states k_n from the $V_\square = 23$ MeV, $R_\square = 7$ fm square well and the eigenvalues, q_ν, from the $V_\square = 28$ MeV well used as the perturbed system in Sec. V.

k_n (fm^{-1})		Energy (MeV)		q_ν (fm^{-1})		Energy (MeV)	
Re	Im	Re	Im	Re	Im	Re	Im
0.000	0.972	−19.758	0.000	0.000	1.086	−24.679	0.000
0.000	−0.909	−17.272	0.000	0.000	−1.037	−22.463	0.000
0.000	0.703	−10.340	0.000	0.000	0.845	−14.945	0.000
0.368	−0.149	2.377	−2.289	0.000	−0.454	−4.316	0.000
1.153	−0.184	27.096	−8.866	0.000	0.176	−0.648	0.000
1.712	−0.213	60.313	−15.213	1.046	−0.173	22.264	−7.580
2.222	−0.237	102.009	−21.984	1.642	−0.201	55.503	−13.809

of the $V_\square = 23$ MeV square well (see Table I) and we show the convergence as a function of the number of a, b, and d states included (although the c states are of course also included). In Fig. 5(a) we also show the expansions

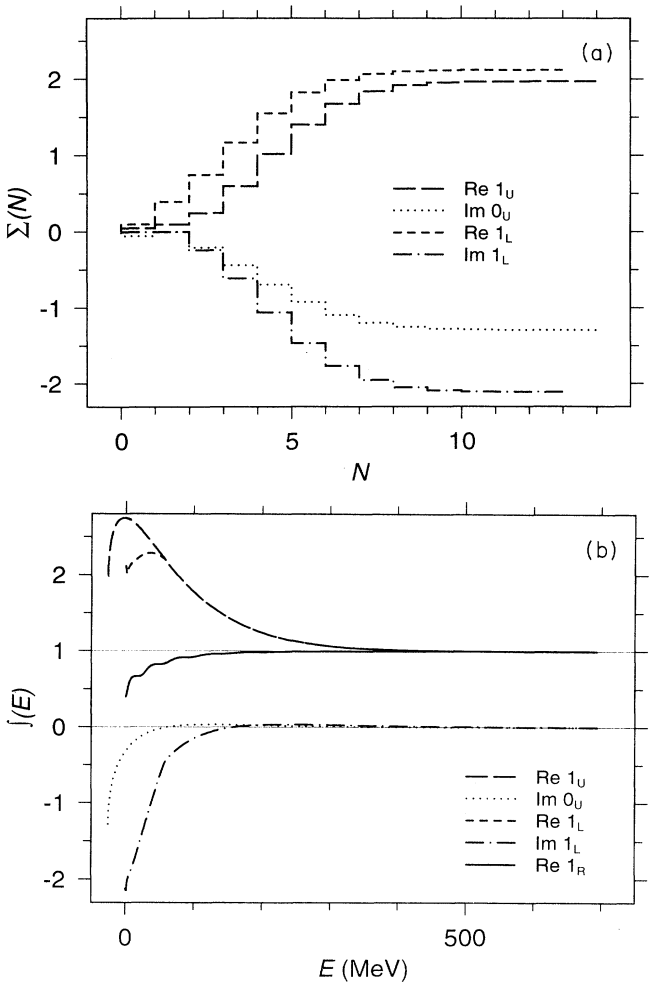

FIG. 4. Resonant state expansions of the matrix element $\langle f|f\rangle = \langle f|\mathbb{1}|f\rangle$ and the expansion $\langle f|\mathbb{O}|f\rangle = 0$, where $f(r)$ is a Gaussian form factor peaked just inside the radius of the square well potential used to generate the basis functions (the $V_\square = 23$ MeV states of Table I). The expansions corresponding to the unit operators (27), (30), and (33) are denoted by 1_R, 1_L, and 1_U, respectively and the zero operator (35) is denoted by 0_U. (a) Discrete part of the expansions as function of the number of $a, b,$ and d states included. The states are ordered according to increasing real part of the energy (as in Table I) and thus the two first steps in the 1_L curves give the contributions from the two bound states to the expansions 1_R and 1_L. In the U expansions there is an antibound state between the bound states. The eleventh (d) resonance has an energy of $631 - 79i$ MeV. (b) Continuum integral contribution to the expansions as function of the upper limit of the parametrized complex contour integrals along the contours R, L, and U. The integrals are performed in the k plane but the upper limit is given here as (real part of) energy. The contributions do not start from 0 but from the final values of the discrete parts in (a).

$\frac{1}{2}\sum_n \langle\mu|f|n\rangle\langle\tilde{n}|f|\nu\rangle \to \langle\mu|f^2|\nu\rangle$ and $\sum_n \frac{\langle\mu|f|n\rangle\langle\tilde{n}|f|\nu\rangle}{2k_n} \to 0$. The expansions in Fig. 5(a) are convergent according to Mittag-Leffler theory. Since the form factor used here is a class T function we are also able to use the expansion (46), and we show in Fig. 5(b) that

$$\sum_{m,n}^{N} \langle\psi_\mu|n\rangle \frac{q_\mu + k_m}{2k_m} \langle\tilde{m}|f^2|n\rangle \frac{q_\nu + k_n}{2k_n} \langle\tilde{n}|\psi_\nu\rangle$$

$$\to \langle\psi_\mu|f^2|\psi_\nu\rangle \ , \ N \to \infty. \quad (53)$$

We also show in this figure that the expansions $\frac{1}{4}\sum_{m,n}\langle\mu|n\rangle\langle\tilde{m}|f^2|n\rangle\langle\tilde{n}|\nu\rangle$ and $\sum_{m,n}\langle\mu|n\rangle\frac{\langle\tilde{m}|f^2|n\rangle}{4k_m k_n}\langle\tilde{n}|\nu\rangle$ do *not* converge to $\langle\mu|f^2|\nu\rangle$ and 0, respectively. The expansion (53) involves radial integrals, $\langle\mu|n\rangle$, where the upper limit is ∞ so this cannot be achieved within the framework of Mittag-Leffler theory. According to that theory we have to do the substitution $\langle\mu|n\rangle \to \langle\mu|P|n\rangle$ but we do not believe that this double expansion should converge [see Fig. 5(b)], since the Mittag-Leffler expansion of a function only converges weakly (see Sec. II C).

4. Expansions of resolvent

We will here illuminate the question of what the continuum background looks like and how it is represented in a resonant state expansion. Since the continuum is related to the integral term in the expansions (47) and (49), we choose to study the single particle response function

$$R_\ell(q) = \langle f|\mathcal{G}_\ell(q)|f\rangle \quad (54)$$

when the form factor f extends considerably beyond the cutoff radius of the potential used to generate the basis functions of the expansions. If we choose a form factor with exponential asymptotics $f(r) \to e^{-\alpha r}$, $r \to \infty$ (such as, e.g., the derivative of a Woods-Saxon potential) we saw in Sec. IV A that the U integral is equal to a closed integral around $k = -i\alpha$. One can then show that

$$\int_U \frac{\langle\tilde{u}_\ell(k)|f\rangle^2}{k(q-k)}\,dk = \frac{\rho_1}{q+i\alpha} + \frac{\rho_2}{(q+i\alpha)^2}, \quad (55)$$

where the complex constants ρ_1 and ρ_2 depend on the integrals $\oint_{k=-i\alpha}\langle\tilde{u}_\ell(k)|f\rangle\,dk$ and $\oint_{k=-i\alpha}\langle\tilde{u}_\ell(k)|f\rangle^2\,dk$. It was found more pedagogical to present numerical results obtained with the same form factor (Gaussian) and basis as used in Sec. IV D 1.

In Fig. 6 we show the response functions obtained with the exact resolvent (11), the L contour expansion (47), and the U contour expansion (49). The expansions are divided into three parts: the discrete part including the states of Table I up to (and including) the third resonance (60 MeV), the rest of the discrete part, i.e., the excluded resonances with energies higher than 100 MeV, and the continuum integral part.

We see that the continuum integral gives a very smooth background (without any resonant features) of the same shape as obtained with an exponential form factor (55). The position of the peak of the form factor was of course chosen so that this contribution is significant. By varying

TABLE II. Values of (1000×) the integrals $-\oint_{k=-q_1}$ (lower triangle) and $-\oint_{k=-q_2}$ (upper triangle) in the expansion of $\langle\tilde{\phi}_1|\phi_2\rangle$, Eq. (42), when the basis is chosen as the $V_\square = 23$ MeV square well states in Table I. The states ϕ_i are chosen from the $V_\square = 28$ MeV square well states and we use one state of each kind: $q_b = 0.176i$, $q_a = -0.454i$, and $q_d = 1.046 - 0.173i$ (fm^{-1}).

		q_2	
q_1	q_b	q_a	q_d
q_b	280	−318	−7.5−i40
q_a	−438	216	−20 −i34
q_d	−13 +i10	20 −i0.4	588 +i59

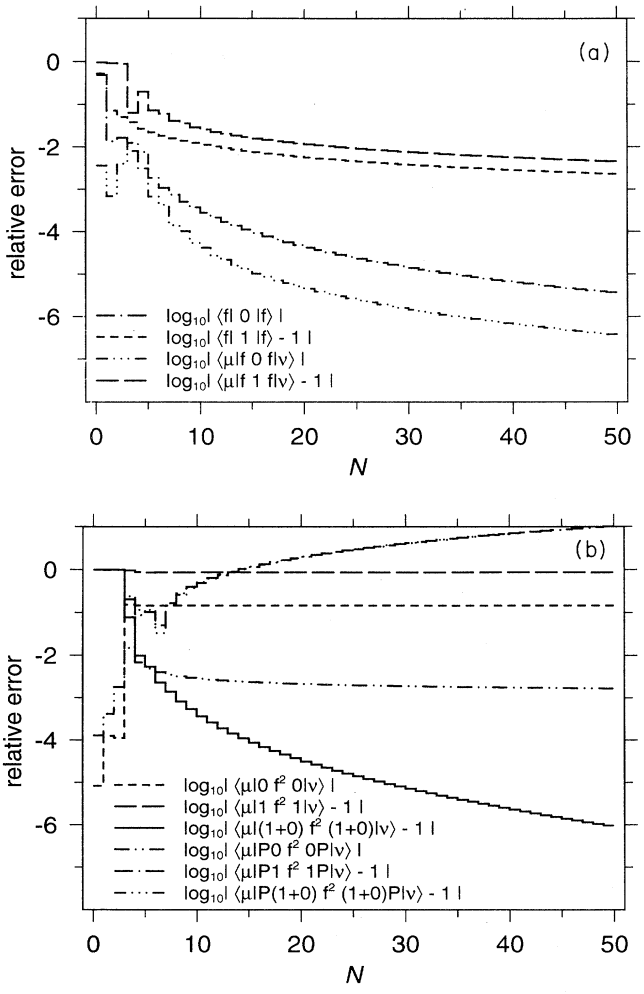

FIG. 5. Logarithm of the relative error (or the logarithm of the expansion in the cases where it converges to zero) as a function of the number of a, b, and d states included in the sum. The basis states are ordered according to increasing real part of the energy as in Table I. (a) Resonant state expansions of the matrix elements $\langle f|f\rangle = \langle f|\mathbb{1}|f\rangle$ and $\langle\psi_\mu|f^2|\psi_\nu\rangle = \langle\psi_\mu|f\mathbb{1}f|\psi_\nu\rangle$ and the corresponding expansions with $\mathbb{1}$ replaced by $\mathbf{O}$ where $\mathbb{1} = \frac{1}{2}\sum_n |n\rangle\langle\tilde{n}|$ and $\mathbf{O} = \sum_n \frac{|n\rangle\langle\tilde{n}|}{2k_n}$. (b) Here we show that we cannot expand $\langle\psi_\mu|f^2|\psi_\nu\rangle = \langle\psi_\mu|\mathbb{1}f^2\mathbb{1}|\psi_\nu\rangle$ but instead should use the expansions (46) and we also show that the corresponding Mittag-Leffler expansions, with $\langle\mu|n\rangle$ replaced by $\langle\mu|P|n\rangle$, do not converge, even if $f = Pf$.

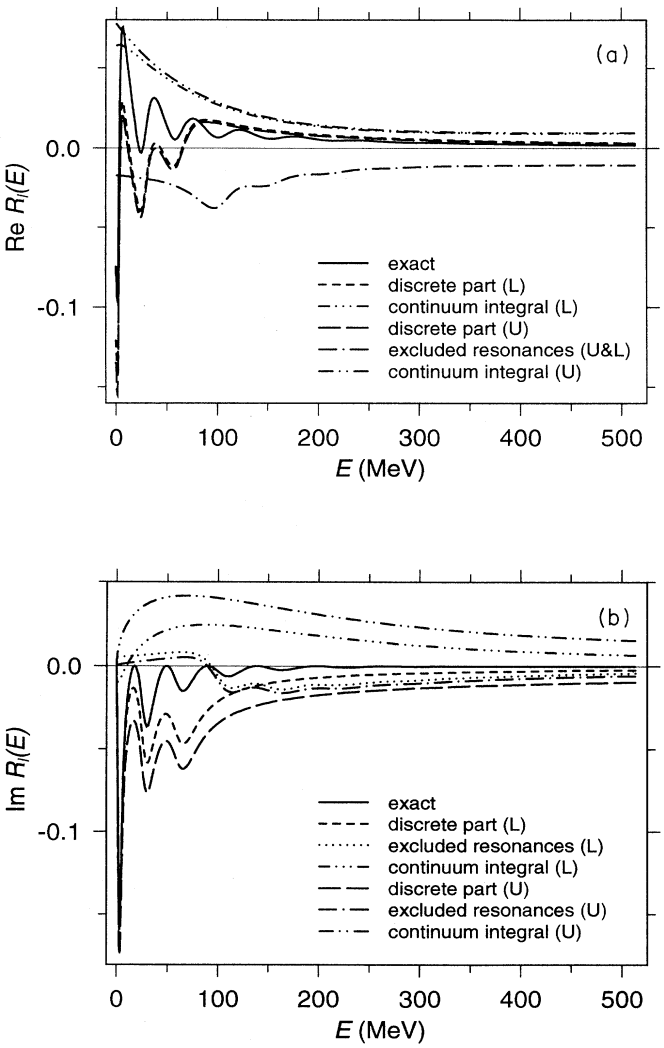

FIG. 6. Resonant state expansions of the resolvent used to calculate the single particle response function $R_\ell(E)$ (in arbitrary units). We show the results when using the exact resolvent (11) and the expansions (47) and (49) corresponding to the L and the U contours, respectively. The contributions from the expansions are divided into three parts that add up to the exact result: the discrete part with states below 100 MeV, the excluded resonances (energies above 100 MeV) and the continuum integral part. We use the basis of Table I. The resonances give equal contributions to the real part of the expansions. (a) Real parts. (b) Imaginary parts.

the shape of the form factor we found in many cases that the continuum integral in the L expansion is smaller than in the U expansion. This is opposite to the case when the form factor is negligible outside the cutoff radius and the U integral vanishes but the L integral does not.

In the contribution from the excluded (high-energy) resonances we see the fourth resonance ($102 - 22i$ MeV), but what is more important is that we see a large background even in the low-energy region.

Because of the substantial low-energy background created by the integral term and the high-energy resonances, the discrete part with all the interesting low-energy states included is clearly insufficient although all the peaks are there. This is in contrast to the realistic case of using Woods-Saxon wave functions and a form factor that is negligible outside the cutoff radius. In this realistic case the low-energy region is very accurately reproduced if all states below 100 MeV are included [24]. Here we chose to present the more artificial example to show that we have a theory that works also formally. We have not emphasized the importance of including unphysical and virtual resonances in order to get a proper representation of the background but this is done in Refs. [11] and [24], especially in the latter.

Similar model studies of the response function have been made [22] with a square well potential and a square barrier form factor, i.e., a function that has a constant value when $|r - 6.75| < 0.75$ and is zero otherwise. This form factor also extends considerably beyond the square well radius ($R_\square = 7$ fm also in that case) and a large background was missing but it was not related to the breaking of the Mittag-Leffler conditions. Improved results were obtained when the form factor was shifted inside the square well radius [25].

V. PERTURBATION PROBLEMS

In this section we give an example of how to use the states in the completeness relations of Sec. III as a basis when solving a differential equation. We study here the perturbed eigenvalue problem

$$({q_\nu}^2 - \mathcal{H}_\ell - V_\lambda)|\psi_\nu\rangle = 0, \tag{56}$$

where $\mathcal{H}_\ell$ is the radial Hamiltonian introduced in Eq. (7) and $V_\lambda(r)$ is the perturbation. The solutions of the unperturbed eigenvalue problem (12) are known and their completeness properties were studied above. We consider perturbations such that there is a one-to-one correspondence between the perturbed and the unperturbed eigenvalues. This is thus the problem treated in elementary quantum mechanics textbooks in terms of perturbation theory although one is then restricted to bound states only. The perturbation expansions are derived using a resolution of the unity in terms of the solutions of Eq. (12), which can also be used to define the "exact" solution, the only source of inaccuracy being the need to use a finite number of states from the complete set.

If we wish to have a perturbation expansion also for resonance and antibound eigenvalues (a continuum perturbation theory), it has been found necessary to start instead from the Dyson equation. We show below how to formulate also an exact procedure from this equation that yields *all* the perturbed eigenvalues of Eq. (56), including the antibound states. This cannot be achieved with any completeness relation.

A. Diagonalizing the Schrödinger equation

If we take a finite number of states in the completeness relation $\mathbb{1} = \sum_n |n\rangle\langle\tilde{n}|$, we can transfer Eq. (56) to a matrix equation and solve it by diagonalizing the matrix

$$\left(\mathcal{H}_\ell + V_\lambda\right)_{mn} = {k_n}^2\delta_{mn} + \langle\tilde{m}|V_\lambda|n\rangle. \tag{57}$$

The improvement obtained by increasing the basis is in this procedure completely different from that in the perturbation expansion. It is our intention to demonstrate that this procedure can be used to find also the resonance eigenvalues, as long as we start from one of the proper completeness relations of Sec. III that includes resonances. These relations, however, contain an integral part that is essential, and we can treat this in two ways: either we can simply neglect it and use only the discrete states or else we can discretize it, i.e., replace the integral by a sum. We first note that, whereas the discrete states will give a symmetric matrix, $\langle\tilde{m}|\mathcal{H}|n\rangle = \langle\tilde{n}|\mathcal{H}|m\rangle$, the continuum states as written previously do not, since $\psi_\ell^*(k^*, r) = S_\ell^{-1}(k)\psi_\ell(k, r)$. As here we are not explicitly interested in the poles of the integrand, we find it convenient to introduce the modified scattering functions (19) so that the integral part of the completeness relations now can be parametrized and discretized symmetrically

$$\begin{aligned}\frac{1}{\pi}\int_C \psi_\ell(k,r)\psi_\ell^*(k^*,r')\,dk &= \int_{C+} u_\ell(k,r)u_\ell(k,r')\,dk \\ &= \int_0^\infty u_\ell(k(t),r)u_\ell(k(t),r')\;\dot{k}(t)dt \\ &\approx \sum_{i=1}^{Ni} u_\ell(k(t_i),r)u_\ell(k(t_i),r')\;\dot{k}(t_i)\Delta t_i \\ &= \sum_{i=1}^{Ni} u^i(r)u^i(r'),\end{aligned} \tag{58}$$

where $u^i(r) = \sqrt{\dot{k}(t_i)\Delta t_i}u_\ell(k(t_i),r)$. We thus obtain the (complex) symmetric matrix (57) that can be diagonalized with standard routines (e.g., [27]) and the result should improve if we increase the size of the matrix. This can be done by including more resonance states $N_{\rm res}$ or more discretized continuum states, which can be achieved in two ways: by increasing the upper limit N_i (i.e., include states with higher energy) or by decreasing the step length Δt_i in the discretization. For consistency one should, perhaps, correlate the two upper limits so that the truncations are made at the same energy even if the result might improve with an uncorrelated increase of $N_{\rm res}$ and N_i.

B. Diagonalizing the Dyson equation

Corresponding to the Eqs. (56) and (12) we can define two resolvents

$$(q^2 - \mathcal{H}_\ell - V_\lambda)\mathcal{G}_\lambda(q) = \mathbb{1},$$

$$(k^2 - \mathcal{H}_\ell)\mathcal{G}(k) = \mathbb{1}$$

(here omitting the angular momentum index), which are related by the Dyson equation

$$\mathcal{G}_\lambda(q) = \mathcal{G}(q) + \mathcal{G}(q)V_\lambda\mathcal{G}_\lambda(q). \tag{59}$$

The perturbation theory of resonance (and antibound) states [26] is derived with the use of the Mittag-Leffler expansions of the resolvents

$$\mathcal{G}_\lambda(q) = \sum_\nu \frac{|\psi_\nu\rangle\langle\tilde{\psi}_\nu|}{2q_\nu(q-q_\nu)},$$

$$\mathcal{G}(k) = \sum_n \frac{|n\rangle\langle\tilde{n}|}{2k_n(k-k_n)}. \tag{60}$$

There is no need for the integral term of (49) if the perturbation V_λ vanishes outside the range of the cutoff potential included in the operator $\mathcal{H}_\ell$.

We can, however, *not* find a diagonalization procedure as in the preceding subsection for all the perturbed eigenvalues q_ν ($a, b, c,$ and d), since these are based on the use of an idempotent resolution of the unit operator which as we saw above cannot include all kinds of pole states (except if it includes a complicated continuum that cannot be neglected or conveniently approximated). In the Appendix we show that we instead should diagonalize the matrix

$$\Big(K+U\Big)_{mn} = k_n\delta_{mn} + \frac{\langle\tilde{m}|V_\lambda|n\rangle}{2\sqrt{k_m k_n}} \tag{61}$$

with m, n running over all a, b and a finite number ($2N_{\rm res}$) of c, d. (This was also found in Ref. [13] from a variation of a stationary expression but no interpretation could be made of the eigenvectors because of the restrictions on Mittag-Leffler theory.) Making use of the eigenvectors from the diagonalization

$$(q_\nu - K - U)\bar{\phi}_\nu = 0$$

with components $(\bar{\phi}_\nu)_n$, we can write the perturbed resolvent as a matrix

$$G_\lambda(q) = \sum_\nu \frac{\bar{\psi}_\nu\bar{\psi}_\nu^T}{2q_\nu(q-q_\nu)}\ ,\ (\bar{\psi}_\nu)_n = \sqrt{\frac{q_\nu}{k_n}}(\bar{\phi}_\nu)_n.$$

In Sec. IV B we suggested that we might have

$$|\psi_\nu\rangle = \sum_n |n\rangle\frac{k_n+q_\nu}{2k_n}\langle\tilde{n}|\psi_\nu\rangle,$$

at least if we only use this expansion together with class T functions. The perturbing potential belongs to this class, and we find numerically (see Table III) that we indeed seem to have

$$(\bar{\phi}_\nu)_n = \frac{k_n+q_\nu}{2\sqrt{k_n q_\nu}}\langle\tilde{n}|\psi_\nu\rangle,$$

i.e.,

$$(\bar{\psi}_\nu)_n = \frac{k_n+q_\nu}{2k_n}\langle\tilde{n}|\psi_\nu\rangle. \tag{62}$$

Since the vectors $\bar{\phi}_\nu$ are the columns of an orthogonal matrix, we also have the remarkable relations

$$\sum_n \langle\tilde{\psi}_\mu|n\rangle\frac{(k_n+q_\mu)(k_n+q_\nu)}{4k_n\sqrt{q_\mu q_\nu}}\langle\tilde{n}|\psi_\nu\rangle = \delta_{\mu\nu} \tag{63a}$$

and

TABLE III. The result for the third (perturbed) bound state in Table I given by diagonalizations of the matrix (61) with $N_{\rm res} = 3, 6, 12,$ and 24. We give in the first line the wave number eigenvalue (fm^{-1}). The other lines compare the amplitudes $(\bar{\phi}_\nu)_n$ with $\frac{k_n+q_\nu}{2\sqrt{k_n q_\nu}}\langle\tilde{n}|\psi_\nu\rangle$ calculated using the exact q_ν, thus suggesting the relations (62). The numbers n refer to the ordering of the basis states (in order of increasing real part of the energy) as given in Table I.

	$N_{\rm dim}=9$		$N_{\rm dim}=15$		$N_{\rm dim}=27$		$N_{\rm dim}=51$		Exact	
	Re	Im	Re	Im	Re	Im	Re	Im	Re	Im
q_ν		0.185		0.181		0.179		0.178		0.1761
n=1 (b)	0.0164		0.0173		0.0178		0.0184		0.0184	
n=2 (a)		−0.0343		−0.0339		−0.0335		−0.0333		−0.0330
n=3 (b)	−0.0626		−0.0653		−0.0668		−0.0676		−0.0686	
n=4 (d)	0.7125	−0.0691	0.7127	−0.0733	0.7127	−0.0759	0.7126	−0.0774	0.7126	−0.0793
n=5 (d)	0.0264	0.0662	0.0292	0.0643	0.0309	0.0635	0.0318	0.0632	0.0330	0.0628

$$\sum_\nu \langle \tilde{m}|\psi_\nu\rangle \frac{(k_m+q_\nu)(k_n+q_\nu)}{4\sqrt{k_m k_n}q_\nu}\langle\tilde{\psi}_\nu|n\rangle = \delta_{mn}, \quad (63b)$$

which we have not been able to derive in any other way although (63a) is rather similar to (53).

C. Numercial illustrations

1. Energy eigenvalues

To show how this diagonalization procedure works, we use as before the states of the $V_\square = 23$ MeV, $R_\square = 7$ fm square well as the unperturbed basis when solving for the eigenvalues of the $V_\square = 28$ MeV well. This case is interesting because for $\ell = 0$, the perturbed system has one more bound state and one more antibound state than the unperturbed system, i.e., when diagonalizing (57) we have to pass the threshold at which a bound-antibound state pair is created from a pair of resonances. (See Ref. [28] for a discussion of square well pole trajectories.) This third bound state is the hardest to reproduce (although it is a square integrable function), so we only show the results for this eigenvalue. It is interesting to compare with the first order perturbation theory (1PT) result $E_\nu^{(1)} = E_n + \langle\tilde{n}|V_\lambda|n\rangle$ (where $|n\rangle$ is the unperturbed state that becomes $|\nu\rangle$ under the action of the perturbation) even if it cannot cope with the threshold, where the complex energy becomes real. For all the other eigenvalues in this example, the error of 1PT is less than 1%.

In Table IV we show the result (cases BQ) when approximating (29) using various numbers, N_i, of included discretized continuum states (DCS) and upper limits $k_{\max}$, chosen between two consecutive Rek_n of the basis in Table I. The interval $(0, k_{\max})$ was divided into N_i equal bins with k_i in the middle. We note that the result can be rather good even with few DCS, but there are also strong fluctuations. In the limit of a larger interval and more DCS the result becomes more accurate.

We also give the result (cases BDQ) when approximating (30) with the number of resonances, $N_{\rm res}$, chosen consistent with the upper limit $k_{\max}$. Here we approximated the L contour by two straight lines $0 + 0i \to 0.33 - 0.3i \to k_{\max} - 0.3i$ with equal bins within the two parts and comparable bins between them. The results are almost as good as in the BQ case but they are more sensitive to the actual parametrization of the contour. There is also a somewhat reduced numerical accuracy when we use complex continuum states far down in the k plane.

We give also the results (case BD and case BCD) of the approximations of neglecting the contours in (30) and (31), respectively. As commented above, the BD case is seen to give a nonzero imaginary part (of the real bound state energy) that the BCD does not. Neither of these two gives results similar to the exact ones even when we increase the basis. The BD results for the other eigenvalues (both bound and resonant) are similar to 1PT, and thus quite accurate. The approximations BQ and BDQ give the other two bound state eigenvalues better than 1PT with just a few DCS and the BDQ give the resonance eigenvalues better if $N_{\rm dim}$ and $k_{\max}$ is chosen large enough. There have been speculations that the BCD basis should be better than the BD basis as an extension of the bound shell model basis, but we strongly emphasize that this is not so. The neglect of the complicated Z contour and the double counting of the resonance contribution is a severe reduction of completeness properties. Except for threshold properties, the BD basis is reasonably satisfactory, since we in the realistic application are not so interested in the convergence when including more basis states as we are in a reasonable representation with few states.

2. Wave number eigenvalues

In Table III we give the wave number eigenvalue q_ν and in Table IV we give also $\frac{\hbar^2}{2m}{q_\nu}^2$ resulting from di-

TABLE IV. The result (in MeV) for the third (perturbed) bound state given by various diagonalizations of the matrix (57) as indicated in the first column. Both the perturbed states and the basis are from the potentials in Table I. The letter B indicates that the basis contains two bound states, the letter D that it contains $N_{\rm res}$ decaying resonances, and C that also $N_{\rm res}$ capturing resonances are used. The letter Q indicates that the basis also contains N_i discretized continuum states with upper limits $k_{\max} = 1.97$, 3.42, and 6.19 for the cases Q1, Q2, and Q3, respectively. For a consistent energy truncation, we have $N_{\rm res} = 3$ in the Q1 case and $N_{\rm res} = 6$ in the Q2 case. $N_{\rm dim}$ is the dimension of the matrix that was diagonalized. The exact value is $E_\nu = -0.6481$ and the prediction of first order perturbation theory is $-2.463 - 0.148i$. The case ABCD is the result of diagonalizing the matrix (61) suggested in Sec. V B and except in the $N_{\rm dim} = 5$ case, the dimension of the diagonalized matrix was actually $N_{\rm dim} + 1$.

	$N_{\rm dim} = 5$		$N_{\rm dim} = 8$		$N_{\rm dim} = 14$		$N_{\rm dim} = 26$		$N_{\rm dim} = 50$	
Case	Re	Im	Re	Im	Re	Im	Re	Im	Re	Im
BQ1	−3.393		−0.386		−0.642		−0.645		−0.645	
BQ2	−0.695		−1.825		−0.708		−0.659		−0.647	
BQ3	7.041		−2.851		−1.075		−0.853		−0.646	
BDQ1	−2.149	−0.026	−1.310	0.514	−0.585	−0.119	−0.630	−0.004	−0.643	−0.003
BDQ2			−2.102	−0.047	−1.201	0.438	−0.582	−0.057	−0.639	−0.001
BD	−2.149	−0.026	−2.102	−0.047	−2.084	−0.058	−2.074	−0.065	−2.060	−0.079
BCD			3.177		3.175		3.174		3.174	
ABCD	−0.843		−0.717		−0.687		−0.669		−0.659	

agonalizations of the matrix (61), for the same case as studied in Sec. V C 1. Compared with the results of that section, this method gives rather good results even with few resonances in the basis. The convergence when we include more resonances is not as fast as when including more DCS in the other methods but seems more stable. We give in Table III also some numbers that support the relation (62).

VI. SUMMARY AND CONCLUSIONS

In all nuclear physics calculations, it is reasonable to say that the realistic potentials (e.g., Woods-Saxon) are of finite range, i.e., they are vanishing beyond a certain radius, R_C. This means that wave functions of bound states and low-lying excited states are very small outside this radius. Scattering states and unbound states have wave functions that are not decreasing outside this radius and for the latter states, they are even increasing with the distance. If one would like to include the unbound states (d and c) in a calculation, one can proceed in two ways: using Mittag-Leffler theory or eigenfunction theory (as was done in this paper).

In the Mittag-Leffler case one assumes that everything interesting happens at distances smaller than the cutoff radius R_C. One then does not have to treat the diverging functions and can use the set of discrete states to expand physical quantities within the limited radial range. But since these states are not orthogonal in this range, it is sometimes hard to interpret the coefficients of the expansions. The expansions, though, are often faster and more convenient from the numerical point of view and the advantage of them is thus more of mathematical nature than physical.

In the case of the eigenfunction treatment, one uses the fact that the discrete states are orthogonal if the radial integrals are taken to infinity even if this means that one has to use regularization procedures for the unbound states. Because of these regularizations and the fact that we have to leave the safe Hilbert space, it is hard to argue with the same mathematical rigor for the validity of the resonant state expansions obtained. [Expansions such as (30) can be argued for mathematically with the use of the rigged Hilbert space theory [29], but this was not useful as a starting point for us here.] Instead we chose to make numerical calculations to show how the relations of Mittag-Leffler theory can be obtained from the eigenfunction theory and how the cutoff radius affects the eigenfunction expansions.

An important feature of the eigenfunction expansions is that we always have a continuum integral contribution in addition to the sum over the discrete states. In the cases where the discrete part has the same form as in Mittag-Leffler theory, the integral vanishes if the conditions of Mittag-Leffler theory are fulfilled. On the other hand, if the Mittag-Leffler conditions are not fulfilled we need the integral to get a valid expansion. We have here given several examples of when the integral is important and as expected, this is in the cases when we consider a quantity that gets a considerable contribution from the radial region outside the cutoff radius. In the realistic case of a truncated Woods-Saxon potential we do not have many such quantities and therefore the Mittag-Leffler expansions are often appropriate. The drawback is the problem with defining and interpreting many-body wave functions. This is no problem in the eigenfunction theory as long as we start from a proper completeness relation, i.e., we can obtain an idempotent expansion of the unit operator. If we neglect the integral term of this proper completeness relation we get an approximate unit operator and if this includes bound states and decaying resonances, it can be viewed as a generalization of the bound shell model basis (at least in a particle-hole formalism [30, 24]).

In Mittag-Leffler theory one divides the radial space into two parts (inside and outside the cutoff radius), and we have two overcompleteness relations that imply the linear dependence of the discrete states over the finite radial range used. Over the infinite radial interval used in the eigenfunction theory we also have two relations: one proper completeness relation and one proper zero operator. If we continue them analytically we can obtain the Mittag-Leffler relations, since the remaining integrals (over the U contour) vanish when applied to cases where the Mittag-Leffler theory also can be used. We found by studying functions with exponential asymptotics that we have to make simultaneous use of both relations if we want to expand wave functions and calculate the coefficients over the infinite radial range. These wave-function expansions are also valid inside the cutoff radius only but this might as mentioned be sufficient in a realistic case.

Correct threshold behavior is obtained only with the Mittag-Leffler expansions or the more general eigenfunctions expansions (33) and (49) derived from the eigenfunction theory, which also gives a correct treatment of the background. We can divide the contributions to a resonant state expansion into three parts: the bound state contributions, the resonant contribution, and the background, which in turn can get its contribution in two ways: from the far away resonances or from the proper continuum integral. In the realistic case there might be no contribution from the U integral and the Mittag-Leffler expansion is valid and useful as long as we do not have to form overlaps between expanded functions.

Summing up we can say that the discussion of our numerical investigations has clarified what it means to have a complete set of functions. We stress the importance of having an expansion of the unit operator that is idempotent. Such a unit operator expansion can be used to derive resonant state expansions of physical quantities that are convenient to work with both from the physical and from the technical point of view. By analytic continuation of these expansions we obtain new expansions that are even more convenient and even if they are shown to be perfectly valid, they seem to imply an expansion of the unit operator that is not idempotent and therefore the completeness is said to be reduced. Observe though that this does not imply that the basis states are orthogonal. It means instead that the validity of the expansions is somewhat restricted and that it is important to perform integrals and analytical continuations in the right order.

By working simultaneously with theoretical derivations (and speculations) and numerical calculations with high accuracy, it was found that the eigenfunction theory behaves well when continued in the complex plane. It might now then be the proper time for a more extensive use of the eigenfunction theory in realistic cases, especially since the conditions there are more advantageous than in this model case [24].

The author is grateful to Tore Berggren for many discussions and to the Swedish Natural Science Research Council for financial support.

APPENDIX: THE MATRIX DYSON EQUATION

We want to solve the perturbed eigenvalue problem (56) using the known basis obtained from the unperturbed eigenvalue problem (12) and the expansion of the (unperturbed) resolvent in terms of the eigenstates and eigenvalues (60).

We first define some matrices by their matrix elements and give some of their properties

$$(G_\lambda)_{mn} = \langle\tilde{m}|\mathcal{G}_\lambda|n\rangle,$$
$$X_{mn} = \langle\tilde{m}|V\mathcal{G}_\lambda|n\rangle,$$

$$G_{mn} = \frac{\delta_{mn}}{2k_n(k-k_n)}, \quad G = (2K)^{-1}(qI-K)^{-1},$$
$$K_{mn} = k_n\delta_{mn},$$

$$T_{mn} = \sqrt{2k_n}\delta_{mn}, \quad T^2 = 2K,$$
$$Q_{\mu\nu} = q_\nu\delta_{\mu\nu},$$

$$S_{\mu\nu} = \sqrt{2q_\nu}\delta_{\mu\nu}, \quad S^2 = 2Q,$$
$$V_{mn} = \langle\tilde{m}|V|n\rangle, \quad V^{\mathrm{T}} = V,$$

$$M_{mn} = \frac{V_{mn}}{2k_n(k-k_n)}, \quad M = VG,$$

$$U_{mn} = \frac{V_{mn}}{2\sqrt{k_m}\sqrt{k_n}}, \quad U = T^{-1}M(qI-K)T,$$

where V^{T} is the transpose of the matrix V and I is the unity matrix, $I_{mn} = \delta_{mn}$. By taking matrix elements between $\langle\tilde{m}|$ and $|n\rangle$ of the Dyson equation (59) by itself and multiplied by V, we get two equations in matrix space

$$G_\lambda = G[I+X], \tag{A1a}$$

$$[I-M]X = M, \tag{A1b}$$

from which we find the perturbed eigenvalues q_ν as the singularities of X, i.e., of $[I-M]^{-1}$ and the residues of G_λ would then be the perturbed eigenvectors expressed in matrix space. [Observe that the transformation from the operator Eq. (59) to the matrix equations (A1a) and (A1b) is done *without* the use of a projection operator of the form $\mathbb{1} = \sum_n |n\rangle\langle\tilde{n}|$ although the use of such an operator would lead to $\mathcal{G}V\mathbb{1}\mathcal{G}_\lambda \to M^{\mathrm{T}}G_\lambda$ (since both V and G are symmetric) and the matrix Dyson equation $[I-M^{\mathrm{T}}]G_\lambda = G$.] The perturbed eigenvalues are thus found by solving

$$\begin{aligned} 0 &= \det\Big[I-M\Big] = \det\Big[I-VT^{-1}(q-K)^{-1}T^{-1}\Big] \\ &= \det\Big[T[I-T^{-1}VT^{-1}(q-K)^{-1}]T^{-1}\Big] \\ &= \det\Big[I-U(q-K)^{-1}\Big], \end{aligned} \tag{A2}$$

i.e., $0 = \det[q-K-U]$, which is the secular equation of the eigenvalue problem

$$[q_\nu - K - U]\bar{\phi}_\nu = 0. \tag{A3}$$

To see why this is relevant, we multiply the second matrix equation (A1b) by T^{-1} and rewrite

$$\begin{aligned} T^{-1}M &= T^{-1}[I-M]X \\ &= T^{-1}[q-K-M(q-K)](q-K)^{-1}X \\ &= [q-K-T^{-1}M(q-K)T]T^{-1}(q-K)^{-1}X \\ &= [q-K-U]T^{-1}(q-K)^{-1}X \end{aligned} \tag{A4}$$

and get an expression for the X matrix

$$X = (q-K)T[q-K-U]^{-1}T^{-1}M. \tag{A5}$$

We can find the inverse $\Gamma = [q-K-U]^{-1}$ by first diagonalizing the symmetric matrix $K+U$ by an orthogonal, $\Phi^{-1} = \Phi^{\mathrm{T}}$, similarity transformation

$$\Phi^{\mathrm{T}}[K+U]\Phi = Q, \tag{A6}$$

where the columns of $\Phi = [\bar{\phi}_1\bar{\phi}_2\cdots]$ is a set of orthogonal, ($\bar{\phi}_\mu^{\mathrm{T}}\bar{\phi}_\nu = \delta_{\mu\nu}$) eigenvectors. The inverse can now be written

$$\Gamma = \Phi[q-Q]^{-1}\Phi^{\mathrm{T}} = \sum_\nu \frac{\bar{\phi}_\nu\bar{\phi}_\nu^{\mathrm{T}}}{q-q_\nu} \tag{A7}$$

and the resolvent (A1a)

$$\begin{aligned} G_\lambda &= G[I+X] \\ &= G(q-K)T\Gamma T^{-1}[T\Gamma^{-1}T^{-1}(q-K)^{-1}+M] \\ &= (2K)^{-1}T\Gamma T^{-1}[I-M+M] = T^{-1}\Gamma T^{-1} \\ &= T^{-1}\Phi[q-Q]^{-1}\Phi^{\mathrm{T}}T^{-1}. \end{aligned} \tag{A8}$$

Making use of the matrix S,

$$[q-Q]^{-1} = S^{-1}2Q[q-Q]^{-1}S^{-1}, \tag{A9}$$

and introducing

$$\Psi = T^{-1}\Phi S = [\bar{\psi}_1\bar{\psi}_2\cdots] \tag{A10}$$

we get

$$G_\lambda = \Psi[2Q(q-Q)]^{-1}\Psi^{\mathrm{T}} = \sum_\nu \frac{\bar{\psi}_\nu\bar{\psi}_\nu^{\mathrm{T}}}{2q_\nu(q-q_\nu)}, \tag{A11}$$

where the components of the vectors in the numerator

are related to the eigenvectors from the diagonalization by

$$(\bar{\psi}_\nu)_n = \sqrt{\frac{q_\nu}{k_n}}(\bar{\phi}_\nu)_n. \tag{A12}$$

We shall not be tempted to identify the coefficient $(\bar{\psi}_\nu)_n$ with the overlap $\langle\tilde{n}|\psi_\nu\rangle$, since the former is of order unity and the latter looks like $\langle\tilde{n}|\nu\rangle = \int_{n\nu} + \frac{N_n N_\nu}{-i(k_n+q_\nu)} e^{i(k_n+q_\nu)R}$, which is not limited.

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