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Resonant states in momentum representation

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Gamow states in momentum representation are defined as solutions of a homogeneous Lippmann-Schwinger equation for purely outgoing particles. We study their properties when the potential, local or nonlocal, is such that the trace of the kernel of the Lippmann-Schwinger equation exists. It is found that, contrary to what happens in position representation, Gamow states in momentum representation are square integrable functions. A norm is defined and expressions for matrix elements of operators between arbitrary states and properly normalized resonant states are given, free of divergence difficulties. It is also shown that bound and resonant states form a biorthonormal set of functions with their adjoints and that a square integrable function may be expanded in terms of a set containing bound states, resonant states, and a continuum of scattering functions. Resonant states may be transformed from momentum to position representation modifying, in a suitable way, the usual rule.

I. INTRODUCTION

It has been appreciated for many years that there are distinct advantages to performing nuclear scattering calculations in momentum space, since many physical effects are then readily expressed and evaluated. In this paper, we intend to show that it is possible to work with Gamow states in momentum representation.

In 1928, Gamow[1] described the α decay of radioactive nuclei with the help of solutions of the Schrödinger equation, which behave at large separation distances as pure outgoing waves and belong to complex eigenvalues. Since then, the possibility of using these resonant eigenstates to describe long lived unbound states and resonances, in nuclear physics and other fields, has been the subject of many investigations.[2,3]

Gamow functions have been widely used in the formal theory of nuclear reactions[4–7] and in the extension to the continuum of the nuclear shell model.[8] More recently, its applications have been extended to the nuclear cluster model of collisions and reactions of light nuclei.[9–11] A numerical procedure for solving, in momentum space, the Coulomb plus nuclear problem for coupled bound and continuum eigenstates was proposed by Landau.[13] A major difficulty in using these functions in practical applications is caused by the fact that a decaying state in position representation is not confined to a finite volume of space. Therefore, its function, the Gamow function, is a wave of exponentially increasing amplitude, which is not square integrable. A number of methods have been proposed for normalizing Gamow functions by integrating over a finite volume and adding a surface term,[14,17] or by regularization techniques[12] or analytic continuation.[15,16] Wave functions decreasing asymptotically faster than any exponential can be expanded in a series of resonance eigenfunctions plus an integral over the complex continuous spectrum.[17]

Since Gamow functions in r representation are not square integrable, the integral that would give its Fourier transform does not exist. However, this does not mean that resonant states do not have a momentum representation, but only that the usual rule for transforming states from position to momentum representation does not apply in this case.

The purpose of this paper is to show that resonance states in momentum representation may be defined as solutions of a homogeneous Lippmann-Schwinger equation appropriate for purely outgoing particle solutions, and to study their properties. The condition of purely outgoing particle solutions makes the problem non-self-adjoint. Therefore, the usual quantum mechanical rules for normalization, orthogonality, and completeness do not apply. It is found that resonant states in momentum representation are square integrable functions. Since resonant states correspond to poles of the transition matrix (t matrix) in unphysical sheets of the complex energy plane,[4,17] Gamow states are related to processes of physical interest through the study of matrix elements of the resolvent operator between arbitrary states. In this way, we define a norm for Gamow states and give expressions for matrix elements of quantum mechanical operators between arbitrary states and properly normalized Gamow states in momentum representation, free of divergence difficulties. The validity of eigenfunction expansions in terms of bound states, resonant states, and a continuum of scattering states is extended to include all square integrable functions. In this paper no claim to mathematical rigor is made.

The plan of the paper is as follows: In Sec. II we state the problem for a potential $U_l(p,p')$ satisfying some suitable conditions. In Sec. III, $U_l(p,p')$ is approximated by a separable potential of rank N_l, with N_l arbitrarily large, and the problem is solved explicitly. The normalization of Gamow states and expressions for matrix elements of quantum mechanical operators between normalized resonant states and arbitrary states in momentum representation are discussed in Sec. IV. In Sec. V, we show that a square integrable function in momentum representation may be expanded in terms of a set of functions containing bound, resonant states and a continuum of scattering functions of complex wave number. These results are illustrated in Sec. VI with a simple example. In Sec. VII we give a summary of our results.

II. RESONANT STATES OF NONLOCAL POTENTIALS IN POSITION AND IN MOMENTUM REPRESENTATION

Let us consider the Schrödinger equation of the relative motion of two nuclear clusters,

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V_d(r)\psi+\int V_e(r,r')\psi(r')d^3r'=E\psi(r)\ . \tag{2.1}$$

Effective equations of this type occur in the description of the scattering of light nuclei in the resonating group method in the one channel approximation[19] and in the microscopic optical potential model description of nucleon-nucleus interactions.[18] In (2.1), r is the position coordinate of the relative motion, $\psi(r)$ is the wave function of the relative motion, and $V_d(r)$ and $V_e(r,r')$ are the direct and exchange potentials. Although there is no difficulty of principle in dealing with the Coulomb interaction, to avoid unnecessary complications, it will not be considered here.

Resonant states in position representation, also called Gamow functions, are solutions of the time independent Schrödinger equation (2.1), which are continuous everywhere and behave as pure outgoing waves for r very large. Solutions of (2.1) which satisfy these conditions exist only for some complex values of the energy with a negative imaginary part.

It may be shown by an elementary argument involving nothing more than the use of the Green's theorem that the Gamow functions $\psi_E(r)$ are also solutions of a homogeneous Lippmann-Schwinger integral equation[20]

$$\psi_E(r)=\int \mathcal{G}_0^{(+)}(\vec{r},\vec{r}\,';k)V(\vec{r}\,',\vec{r}\,'')\psi_E(\vec{r}\,'')d^3r'd^3r''\ . \tag{2.2}$$

In this expression $\mathcal{G}_0^{(+)}(\vec{r},\vec{r}\,';k)$ is the Green's function of a free particle with outgoing wave boundary conditions

$$\mathcal{G}_0^{(+)}(\vec{r},\vec{r}\,';k)=-\frac{m}{2\pi\hbar^2}\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|r-r'|}\ , \tag{2.3}$$

and $V(\vec{r},\vec{r}\,')$ is the sum of the direct and exchange potentials

$$V(\vec{r},\vec{r}\,')=V_d(r)\delta(\vec{r}-\vec{r}\,')+V_e(\vec{r},\vec{r}\,')\ . \tag{2.4}$$

Since the imaginary part of the energy E_n is negative, the wave number k_n also has a negative imaginary part. It follows from (2.2) and (2.3) that Gamow functions are waves of exponentially increasing amplitude for r very large. Hence, they are not square integrable, and the integral that would give their Fourier transform does not exist. This means that the usual rule for transforming quantum mechanical states from position to momentum representation does not apply in this case. On the other hand, when the potential $V(\vec{r},\vec{r}\,')$ has a Fourier transform, there is no difficulty in writing the Lippmann-Schwinger equation in momentum representation. Therefore, resonant states in momentum representation may be obtained as solutions of the homogeneous Lippmann-Schwinger equation for outgoing particles in that representation, corresponding to complex energy eigenvalues.

Before writing the Lippmann-Schwinger equation in momentum representation, it is convenient to note that in the integral equation (2.2), the outgoing wave condition for r very large is imposed on $\psi_E(r)$ through the definition of the free particle's Green's function. This Green's function is the position representation of the resolvent operator of the Hamiltonian of a free particle, and is related to its momentum representation through the spectral representation

$$\mathcal{G}_0^{(+)}(\vec{r},\vec{r}\,';k)=\lim_{\epsilon\to 0}\frac{1}{2\pi\hbar}\int e^{i(\vec{p}\cdot\vec{r}/\hbar)}\frac{1}{E+i\epsilon-\frac{p^2}{2m}}\times e^{-i(\vec{p}\cdot\vec{r}\,'/\hbar)}d^3p\ , \tag{2.5}$$

with E real and ϵ positive. A similar relation holds true for the Green's function for incoming waves, but with a negative imaginary term in the denominator. The integral (2.5), as a function of the energy E, is discontinuous on the real axis. Therefore, when using the spectral representation (2.5) in the integral equation (2.2), the prescription to obtain outgoing wave solutions is to define the integral in the upper half of the energy plane and then to continue it analytically to the lower half plane.

Taking into account the above considerations, the homogeneous Lippmann-Schwinger equation defining resonant states in momentum representation is written as

$$\psi_{E_n}(\vec{p})=\left[\int\int\frac{\delta(\vec{p}-\vec{p}\,')}{E^{(+)}-\frac{p^2}{2m}}V(\vec{p}\,',\vec{p}\,'')\psi_E(p'')d^3p'd^3p''\right]_{E_n}\ . \tag{2.6}$$

$V(\vec{p},\vec{p}\,')$ is the Fourier transform of the potential

$$V(\vec{p},\vec{p}\,')=\frac{1}{(2\pi\hbar)^3}\int\int e^{-i(\vec{p}\cdot\vec{r}/\hbar)}V(r,r')\times e^{i(\vec{p}\,'\cdot\vec{r}\,'/\hbar)}d^3r\,d^3r'\ . \tag{2.7}$$

The notation $E^{(+)}$ and the square brackets in (2.6) mean that the kernel of the integral equation is defined with E in the upper half of the energy plane, then the integration over the momentum variables is performed and the resulting function of the energy E is continued analytically to E_n in the lower half of the energy plane. The order in which these operations are performed is important because just writing E_n in the integrand, with $\mathrm{Im}E_n<0$, would result in a Lippmann-Schwinger equation for purely outgoing particles with a kernel appropriate for purely incoming solutions, which is obviously inconsistent. Integration over $\vec{p}\,'$ in (2.6) gives the Schrödinger equation for Gamow states in momentum representation,

$$\frac{p^2}{2m}\psi_{E_n}(\vec{p})+\left[\int V(\vec{p},\vec{p}\,'')\psi_E(\vec{p}\,'')d^3p''\right]_{E=E_n}=E_n\psi_{E_n}(\vec{p})\ . \tag{2.8}$$

Even when the integral equation defining Gamow states in momentum representation is written as in (2.8), the condition of purely outgoing particle solutions is imposed through the definition of the integral as a function of the energy, as will become apparent from the results of Sec. III.

To simplify the problem it is convenient to make a partial wave expansion. Since the potential is rotationally invariant it may be expanded in spherical harmonics as

$$V(\vec{p},\vec{p}\,')=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\Omega_p)\frac{V_l(p,p')}{pp'}Y^*_{lm}(\Omega_{p'}) \tag{2.9}$$

and a similar expansion for the wave function,

$$\psi_{E_n}(\vec{p})=\sum_{l=0}^{\infty}\sum_{l=-l}^{l}\frac{u_{nl}(p)}{p}Y_{lm}(\Omega_p)\ . \tag{2.10}$$

Insertion of (2.9) and (2.10) in (2.6) gives the Lippmann-Schwinger equation for the partial wave $u_{nl}(p)$,

$$u_{nl}(q;k_n)=\left[\int_0^\infty K_l^{(+)}(q,q';k)u_{nl}(q';k)dq\right]_{k_n}\ . \tag{2.11}$$

In this expression

$$K_l^{(+)}(q,q';k)=\int_0^\infty\frac{\delta(q-q'')}{k^2+i\epsilon-q''^2}U_l(q'',q')dq''\ , \tag{2.12}$$

with k^2 real, ϵ positive,

$$U_l(q,q')=\frac{2m}{\hbar}V_l(q,q')\ ,$$

$$\hbar q=p,\ \text{and}\ k^2=\frac{2mE}{\hbar^2}\ .$$

For spinless particles, the interaction potential $U_l(q,q')$ is real and symmetric.

The conditions for the existence of solutions of the Lippmann-Schwinger equation (2.11) are well known.[21–25] Solutions of (2.11) exist, even when the kernel is infinite at one point, provided that the Fredholm's determinant of $1-K_l^{(+)}$ vanishes,

$$\Delta_l^{(+)}(k)=\det\{\underline{1}-\underline{K}_l^{(+)}(k)\}=0\ , \tag{2.13}$$

and the integrals

$$\int_0^\infty\int_0^\infty|U_l(q,q')|^2dq\,dq'\ , \tag{2.14}$$

$$\int_0^\infty|U_l(q,q')|^2dq'\ , \tag{2.15}$$

with

$$U_l(q,q')=U_l(q',q)\ , \tag{2.16}$$

exist, and the latter, regarded as a function of q, remains below a fixed bound.[22,26]

Fredholm's first minor $M_l(q,q')$ of the kernel $(\underline{1}-\underline{K}_l^{(+)})$ satisfies the integral relation, sometimes called Fredholm's second fundamental relation,[24,25]

$$M_l(q,q';E)=\eta(E)\Delta_l^{(+)}(E)\frac{\delta(q-q')}{k^2-q'^2}+\eta(E)\int_0^\infty\int_0^\infty\frac{\delta(q-q'')}{k^2+i\epsilon-q''^2}U_l(q'',q''')\times M_l(q''',q;E)dq''dq'''\ . \tag{2.17}$$

when E is equal to the complex eigenvalue E_n, $\Delta_l^{(+)}(E_n)$ vanishes, $\eta(E_n)=1$,[23,26,28] and (2.17) reduces to (2.11), showing that $M_l(q,q_0;E_n)$ is a solution of (2.11).

Under the assumptions (2.14)–(2.16) the trace of the kernel $K_l^{(+)}(k)$ exists,[22,24]

$$\sigma_l(k)=\mathrm{tr}[\underline{K}_l^{(+)}(k)]=\int_0^\infty\frac{U_l(q,q)}{k^2+i\sigma-q^2}dq\ . \tag{2.18}$$

In practical applications, the Fredholm determinant and the Fredholm first minor may be evaluated, expanding them as

$$\Delta_l^{(+)}(k)=e^{-\sigma_l(k)}\sum_{m=0}^{\infty}\delta_{lm}(k) \tag{2.19}$$

and

$$M_l(q,q_0;k)=e^{-\sigma_l(k)}\sum_{m=0}^{\infty}\mu_{lm}(q,q_0;k)\ . \tag{2.20}$$

The coefficients $\delta_{lm}(k)$ and $\mu_{lm}(q,q_0;k)$ are then obtained from a suitable set of recursion relations.[21]

III. GAMOW STATES IN A SEPARABLE POTENTIAL

To establish the existence and properties of Gamow states in the momentum representation for a potential satisfying (2.14)–(2.16), it is sufficient to study the solutions of the homogeneous Lippmann-Schwinger equation (2.11) when the potential function is approximated by separable potentials[22,25] (continuous degenerate kernels).

$$U_l(q,q')\simeq U_l^{(N_l)}(q,q')=\sum_{s=1}^{N_l}\sum_{s'=1}^{N_l}f_s^{(l)}(q)v_{ss'}f_{s'}^{(l)*}(q') \tag{3.1}$$

in such a way that the following conditions are satisfied. The integral

$$\int_0^\infty\left|\frac{U_l(q,q')-U_l^{(N_l)}(q,q')}{W-q'^2}\right|^2dq' \tag{3.2}$$

becomes arbitrarily small in q as $N\to\infty$ and the integral

$$\int_0^\infty\frac{U_l^{(N_l)}(s+\epsilon,t)-U_l^{(N_l)}(s,t)}{W-s^2}dt \tag{3.3}$$

becomes arbitrarily small in s and in N_l if ϵ is taken sufficiently small.[27]

The set of linearly independent orthonormal functions $\{f_s^{(l)}(q)\}$ is characterized by requiring that $f_s^{(l)}(q)$ belongs to it, if and only if $f_s^{(l)}(q)$ is a function which can be analytically continued from the real positive axis to the whole of the complex plane, and the resulting continuation is entire. We further require that this set be complete in the Hilbert space of L^2 functions on $[0,\infty)$. An example of such a set is the set of radial eigenfunctions of a three-dimensional harmonic oscillator.

The potential $U_l(q,q')$ is expanded in terms of the set $\{f_s^{(l)}(q)\}$,

$$U_l(q,q')=\sum_{s=1}^{\infty}\sum_{s'=1}^{\infty} f_s^{(l)}(q)v_{ss'}f_{s'}^{(l)*}(q') , \tag{3.4}$$

and the matrix element $v_{ss'}$ of the potential is given by

$$v_{ss'}=\int_0^\infty\int_0^\infty f_s^{(l)*}(q)U_l(q,q')f_{s'}^{(l)}(q')dq\,dq' . \tag{3.5}$$

Next, we approximate $U_l(q,q')$ by the nonlocal separable potential of rank N_l, $U^{(N_l)}(q,q')$, which is obtained from $U_l(q,q')$ truncating the expansion (3.4):

$$U_l^{(N_l)}(q,q')=\sum_{s=1}^{N_l}\sum_{s'=1}^{N_l} f_s^{(l)}(q)v_{ss'}f_{s'}^{(l)*}(q') . \tag{3.6}$$

In this approximation, the Lippmann-Schwinger equation for the lth component, $u_{nl}(q)$, of the resonant state becomes

$$u_{nl}(q;k_n)=\sum_{s=1}^{N_l}\sum_{s'=1}^{N_l}\left[\int_0^\infty \frac{\delta(q-q')}{k^2-q'^2}f_s^{(l)}(q') \times v_{ss'}n_{nls'}(k)\right]_{k_n} , \tag{3.7}$$

where

$$n_{nls}(k)=\int_0^\infty f_s^{(l)*}(q)u_{nls}(q;k)dq . \tag{3.8}$$

The integrals in equations (3.7) and (3.8) are defined with $\mathrm{Im}k>0$ and the resulting functions of k are analytically continued to k_n.

The solution of the integral equations (3.7) and (3.8) may be reduced to the solution of a homogeneous system of N_l coupled linear equations. In order to show this, we expand $u_{nl}(q;k)$ in terms of the set $\{f_s^{(l)}(q)\}$,

$$u_{nl}(q;k)=\sum_{s=1}^{\infty} n_{nls}(k)f_s^{(l)}(q) , \tag{3.9}$$

with $n_{nls}(k)$ given by (3.8), and we insert in (3.7) a $\delta(q-q')$ written as

$$\delta(q-q')=\sum_{s=1}^{\infty} f_s^{(l)}(q)f_s^{(l)*}(q') . \tag{3.10}$$

In this way we obtain

$$\sum_{s=1}^{\infty} f_s^{(l)}(q)\left[n_{nls}(k_n)-\sum_{s'=1}^{N_l}\sum_{s''=1}^{N_l} G_{0lss'}^{(+)}(k_n)v_{s's''}n_{nls''}(k_n)\right]=0 . \tag{3.11}$$

The matrix $\underline{G}_{0l}^{(+)}(k)$ is defined in terms of the Cauchy integral

$$G_{0lss'}^{(+)}(k)=\int_0^\infty f_s^{(l)*}(q)\frac{1}{k^2-q^2}f_{s'}^{(l)}(q)dq \tag{3.12}$$

for $\mathrm{Im}k>0$. The analytic continuation of $G_{0lss'}^{(+)}(k)$ to the lower half of the wave number k plane follows from the Plemelj formulae[24]

$$G_{0lss'}^{(+)}(k)=\int_0^\infty f_s^{(l)*}(q)\frac{1}{k^2-q^2}f_{s'}^{(l)}(q)dq - i\pi\frac{f_s^{(l)*}(k^*)f_{s'}^{(l)}(k)}{k} \tag{3.13}$$

for $\mathrm{Im}k<0$.

Since the $f_s^{(l)}(q)$s are linearly independent, all the coefficients of the $f_s^{(l)}(q)$ that appear in Eq. (3.11) must vanish. Therefore, the expansion coefficients $n_{nls}(k_n)$ satisfy the system of homogeneous linear equations

$$n_{nls}(k_n)=\sum_{s'=1}^{N_l}\sum_{s''=1}^{N_l} G_{0lss'}^{(+)}(k_n)v_{s's''}n_{nls''}(k_n) \tag{3.14}$$

for $1\le s\le N_l$, and the relation

$$n_{nls}(k_n)=\sum_{s'=1}^{N_l}\sum_{s''=1}^{N_l} G_{0lss'}^{(+)}(k_n)v_{s's''}n_{nls''}(k_n) \tag{3.15}$$

for $s>N_l$.

Since relation (3.15) gives the expansion coefficients $n_{nls}(k_n)$ of $u_{nl}(q;k_n)$ with indices s larger than N_l in terms of those with indices s smaller than or equal to N_l, the solutions of the Lippmann-Schwinger equation (3.7) are completely determined by the solutions of the system of homogeneous linear equations (3.14). In matrix notation

$$\underline{n}_{nl}(k_n)=\underline{K}_l^{(+)}(k_n)\underline{n}_{nl}(k_n) . \tag{3.16}$$

The $N_l\times N_l$ matrix $\underline{K}_l^{(+)}(k)$ is

$$K_{lss'}^{(+)}(k)=\sum_{s''=1}^{N_l} G_{0lss''}^{(+)}(k)v_{s''s'} \tag{3.17}$$

with $1\le s\le N_l$ and $1\le s'\le N_l$.

A necessary and sufficient condition for the existence of solutions of (3.16) and, hence, of (3.7) and (3.8), is the vanishing of the determinant $\Delta_l^{(+)}(k)$ of the matrix $(\underline{1}-\underline{K}_l^{(+)}(k))$. The eigenvalues E_n are the roots of the equation

$$\Delta_l^{(+)}(E_n)=0 . \tag{3.18}$$

When $\Delta_l^{(+)}(k)$ has a simple zero at k_n, we may suppose that the rank of $(\underline{1}-\underline{K}_l^{(+)}(k_n))$ is (N_l-1), and let Eqs. (3.14) and also the unknowns $n_{nls}(k_n)$ be arranged so that the leading submatrix of $(\underline{1}-\underline{K}_l^{(+)}(k_n))$ of order (N_l-1) is nonsingular. Let the cofactors of the last row be taken as the elements of a column vector $M_{nls}(k_n)$; then

$$(\underline{1}-\underline{K}_l^{(+)}(k_n))\underline{M}_{nl}(k_n)=0 , \tag{3.19}$$

showing that $\underline{M}_{nl}(k_n)$ is a solution of (3.14) or (3.16). The corresponding solution of the homogeneous Lippmann-Schwinger equation (3.7) is

$$u_{nl}(q;k_n)=\frac{1}{k_n^2-q^2}\sum_{s=1}^{N_l}\sum_{s'=1}^{N_l} f_s^{(l)}(q)v_{ss'}M_{nls'}(k_n) \ . \tag{3.20}$$

A number of properties of the solutions $u_{nl}(q;k_n)$ are readily obtained from the properties of the solutions of (3.16). We notice first that the determinant $\Delta_l^{(+)}(k)$ of the matrix $(\underline{1}-\underline{K}_l^{(+)}(k))$ has properties similar to those of the Jost function of local potentials. Indeed, when $U_l(r)$ is a local potential, $\Delta_l^{(+)}(k)$ is the Jost function.[21] These properties are the following:

(i) As already stated, the vanishing of $\Delta_l^{(+)}(k)$ is a necessary and sufficient condition for the existence of solutions of (3.16) and, hence, of solutions of the homogeneous Lippmann-Schwinger equation (3.7).

(ii) The equation

$$\Delta_l^{(+)}(k)=\Delta_l^{(+)*}(-k^*) \ . \tag{3.21}$$

(iii) The zeros of $\Delta_l^{(+)}(k)$ are located on the imaginary axis and in the lower half of the wave number k plane, including the real axis.

(iv) The resolvent of $H_l^{(N_l)}$ and the collision matrix S_l have poles in the k plane located precisely where $\Delta_l^{(+)}(k)$ has zeros.[29]

Properties (ii) and (iii) follow directly from the analytic properties of the matrix elements $G_{0lss'}^{(+)}(k)$. From equations (3.12) and (3.13) and[30]

$$f_s^{(l)}(-q)=(-1)^l f_s^{(l)}(q) \ , \tag{3.22}$$

it follows that

$$G_{0lss'}^{(+)*}(-k^*)=G_{0ls's}^{(+)}(k) \ , \tag{3.23}$$

and, since the potential $\underline{v}$ is Hermitian and energy independent,

$$K_{lss'}^{(+)*}(-k^*)=K_{ls's}^{(+)}(k) \ . \tag{3.24}$$

From (3.24), (3.21) follows immediately. Although (iii) and (iv) are well known,[21,23] for the sake of completeness, we give an elementary derivation of them in the Appendix.

We will now introduce the adjoint $\tilde{u}_{nl}(q;k_n)$ of a Gamow state $u_{nl}(q;k_n)$ as the left solution of the integral equation (2.11) that belongs to the same eigenvalue E_n.

From (3.17) and (3.24), we get

$$n_{nls}^*(-k_n^*)=\sum_{s''=1}^{N_l} n_{nls''}^*(-k_n^*)K_{ls''s}^{(+)}(k_n) \ , \tag{3.25}$$

that is, $n_{nls}^*(-k_n^*)$ is a left eigenvector of $\underline{K}_l^{(+)}$ that belongs to the same eigenvalue k_n as $\underline{n}_n(k_n)$. This relation suggests taking the complex conjugate of Eq. (2.11):

$$u_{nl}^*(q;k_n)=\left[\int_0^\infty\int_0^\infty \frac{\delta(q-q')}{k^{*2}-q'^2}U_l^*(q',q'') \times u_{nl}^*(q''k)dq'dq''\right]_{k_n^*} .$$

Recalling that $U_l(q,q')$ is Hermitian and $\delta(q-q')$ is symmetric, and substituting $-k^*$ for k, this equation may be rearranged to give

$$u_{nl}^*(q;-k_n^*)=\left[\int_0^\infty\int_0^\infty u_{nl}^*(q'';-k^*)U_l(q'',q') \times \frac{\delta(q'-q)}{k^2-q'^2}dq\,dq'\right]_{k_n} , \tag{3.26}$$

showing that the adjoint $\tilde{u}_{nl}(q;k_n)$ of $u_{nl}(q;k_n)$ is given by

$$\tilde{u}_{nl}(q;k_n)=u_{nl}^*(q;-k_n^*) \ . \tag{3.27}$$

In the case of interactions between spinless particles, the potential $U_l(q,q')$ is a real function, symmetric in its arguments. We can make use of this property to rewrite Eq. (3.26) as

$$\tilde{u}_{nl}(q;k_n)=\left[\int_0^\infty\int_0^\infty \frac{\delta(q-q')}{k^2-q'^2}U_l(q',q'') \times \tilde{u}_{nl}(q'';k)dq'dq''\right]_{k_n} , \tag{3.28}$$

which is the same equation as (2.11). Therefore, for spinless particles, $\tilde{u}_{nl}(q;k_n)$ is proportional to its adjoint. Without any loss of generality, we may write

$$\tilde{u}_{nl}(q;k_n)=u_{nl}(q;k_n) \ . \tag{3.29}$$

It is now easy to prove an orthogonality relation for bound and resonant states. From (3.27) and (3.29), we obtain

$$u_{nl}(q;k_n)=\sum_{s=1}^{N_l}\sum_{s'=1}^{N_l} n_{nls}^*(-k_n^*)v_{ss'}f_{s'}^{(l)*}(q)\frac{1}{k_n^2-q^2} \ , \tag{3.30}$$

and from this equation and the definition of $G_{0l}^{(+)}(k)$, a straightforward calculation yields

$$\int_0^\infty u_{nl}(q;k)u_{n'l}(q;k')dq=\frac{1}{k'^2-k^2}\{\underline{n}_{nl}^\dagger(-k^*)\underline{v}[\underline{G}_{0l}^{(+)}(k)-\underline{G}_{0l}^{(+)}(k')]\underline{v}\,\underline{n}_{nl}(k')\} \ ,$$

with k and k' in the upper half plane. Now, we take the limit $k\to k_n$ and $k'\to k_{n'}$ with $k_{n'}\neq k_n$, and make use of (3.16) and (3.25),

$$\left[\int_0^\infty u_{nl}(q;k)u_{n'l}(q;k')dq\right]_{\substack{k=k_n\\k'=k_{n'}}}=0 \ . \tag{3.31}$$

Taking the same limit with $k_n=k_{n'}$ yields

$$\left[\int_0^\infty u_{nl}(q;k)u_{nl}(q;k)dq\right]=\frac{1}{2k_n}\underline{n}_{nl}^\dagger(-k_n^*)\underline{v}\left[\frac{d(\underline{1}-\underline{K}_l^{(+)}(k))}{dk}\right]_{k_n}\underline{n}_{nl}(k_n) \ . \tag{3.32}$$

Collecting these results in one formula,

$$\left[\int_0^\infty u_{nl}(q;k)u_{n'l}(q;k')dq \right]_{\substack{k=k_n\\k'=k_{n'}}} = -\delta_{nn'}\frac{1}{2k_n}\underline{n}^\dagger_{nl}(-k_n^*)\underline{v}\left[\frac{d\underline{G}_{0l}^{(+)}(k)}{dk}\right]_{k_n}\underline{v}\,\underline{n}_{nl}(k_n)\,. \tag{3.33}$$

When $u_{nl}(q;k_n)$ is a real bound state wave function, E_n is real and negative, k_n is imaginary, and Eq. (3.33) reduces to the usual orthogonality relation for bound states. However, for Gamow states the wave function $u_{nl}(q;k)$ is complex, and it is equal to its adjoint; therefore, in this case Eq. (3.33) differs from the usual orthogonality relation for eigenfunctions with real eigenvalues.

A convenient way to relate the integral appearing in (3.33) with processes of physical interest is provided by the study of the Green's operator for outgoing particles.[17]

In what follows we examine the behavior of the resolvent of H_l near one of its complex poles. It will be shown that the residue of the resolvent of H_l at the pole k_n is proportional to the inverse of the integral that appears on the left-hand side of (3.33).

The restriction to the lth wave of the resolvent of H_l satisfies the integral equation

$$\left\langle q \left| \frac{1}{E^{(+)}-H_l} \right| q' \right\rangle = \frac{\delta(q-q')}{k^2-q'^2} + \int_0^\infty \int_0^\infty \frac{\delta(q-q'')}{k^{2(+)}-q''^2} U_l(q'',q''') \left\langle q''' \left| \frac{1}{E^{(+)}-H_l} \right| q' \right\rangle dq''dq''' \,, \tag{3.34}$$

where

$$\left\langle q \left| \frac{1}{E^{(+)}-H_l} \right| q' \right\rangle = \frac{\hbar^3}{2m} \left\langle p \left| \frac{1}{E^{(+)}-H_l} \right| p' \right\rangle .$$

When $U_l(q,q')$ is approximated by a separable potential $U_l^{(N_l)}(q,q')$, the integral equation (3.34) may be readily solved to yield

$$\left\langle q \left| \frac{1}{E^{(+)}-H_l^{(N_l)}} \right| q' \right\rangle = \frac{\delta(q-q')}{k^{2(+)}-q'^2} + \sum_{s=1}^{N_l}\sum_{s'=1}^{N_l} \frac{1}{k^{2(+)}-q^2} f_s^{(l)}(q)[(\underline{A}_l^{(+)}(k))^{-1}]_{ss'} f_{s'}^{(l)*}(q')\frac{1}{k^2-q'^2}\,. \tag{3.35}$$

The matrix $\underline{A}_l^{(+)}(k)$ that appears in this expression is given by

$$\underline{A}_l^{(+)}(k) = (\underline{1}-\underline{K}_l^{(+)}(k))\underline{v}^{-1}\,. \tag{3.36}$$

Since the first term on the right-hand side of (3.35) is analytic at E_n, to study the behavior of the resolvent near one of its complex poles we must study $(\underline{A}_l^{(+)}(k))^{-1}$ in the vicinity of E_n.

Let us notice first that

$$\det[\underline{A}_l^{(+)}(k)] = (\det\underline{v})^{-1}\Delta_l^{(+)}(k)\,. \tag{3.37}$$

Let us suppose that the zero of $\Delta_l^{(+)}(k)$ at E_n is simple; then, since $\underline{v}$ is independent of the energy, $\det\underline{A}_l^{(+)}(k)$ has a simple zero at E_n. We expand $(\underline{A}_l^{(+)}(k))^{-1}$ in terms of the left $\underline{\tilde{m}}_\mu$ and right $\underline{m}_\mu$ eigenvectors of $\underline{A}_l^{(+)}(k)$; then

$$(\underline{A}_l^{(+)})^{-1} = \sum_{\mu=1}^{N_l} \underline{m}_\mu(E)\frac{1}{a_\mu(E)}\underline{\tilde{m}}_\mu(E)\,. \tag{3.38}$$

From (3.36) and (3.16), it follows that one of the eigenvalues of $\underline{A}_l^{(+)}(E)$, say $a_1(E)$, goes to zero when E goes to E_n, while the corresponding right and left eigenvectors go to $\underline{v}\,\underline{n}_{nl}(E_n)$ and $\underline{\tilde{n}}_{nl}(E_n)\underline{v}$, respectively, and, since we assumed that the zero of $\underline{A}_l^{(+)}(E)$ at E_n is simple, all the other eigenvalues are nonzero at E_n,

$$a_1(E) \simeq (E-E_n)\underline{\tilde{n}}_{nl}(E_n)\underline{v}\left[\frac{d\underline{A}_l^{(+)}(E)}{dE}\right]_{E_n}\underline{v}\,\underline{n}_{nl}(E_n)$$

$$+O(|E-E_n|^2)$$

and

$$a_\mu(E) \simeq \underline{\tilde{m}}_\mu(E_n)\underline{A}_l^{(+)}(E_n)\underline{m}_\mu(E_n) + O(|E-E_n|) \quad \mu\neq 1\,.$$

From these relations we obtain

$$\lim_{E\to E_n}(E-E_n)(\underline{A}_l^{(+)}(E))^{-1} = \underline{v}\,\underline{n}_{nl}(E_n)\frac{1}{\underline{\tilde{n}}_{nl}(E_n)\underline{v}\left[\dfrac{d\underline{A}_l^{(+)}}{dE}\right]_{E_n}\underline{v}\,\underline{n}_{nl}(E_n)}\underline{\tilde{n}}_{nl}(E_n)\underline{v}\,. \tag{3.39}$$

Recalling (3.36) and (3.17), we obtain

$$\frac{d\underline{A}_l^{(+)}(E)}{dE} = -\frac{d\underline{G}_{0l}^{(+)}(E)}{dE}\,. \tag{3.40}$$

From this result and Eqs. (3.33) and (3.25), it follows that

$$\lim_{E\to E_n}(E-E_n)(\underline{A}_l^{(+)}(E))^{-1}=\underline{v}\,\underline{n}_{nl}(k_n)\frac{1}{\left[\int_0^\infty u_{nl}^2(q;k)dq\right]_{k_n}}\tilde{\underline{n}}_{nl}(k_n)\underline{v}\ . \tag{3.41}$$

Therefore,

$$\lim_{E\to E_n}(E-E_n)\left\langle q\left|\frac{1}{E^{(+)}-H_l}\right|q'\right\rangle=u_{nl}(q;k_n)\frac{1}{\left[\int_0^\infty u_{nl}^2(q;k)dq\right]_{k_n}}u_{nl}(q';k_n)\ . \tag{3.42}$$

IV. NORMALIZATION OF GAMOW STATES

The resolvent operator occurs in the calculation of transition amplitudes and cross sections in matrix elements which, in the approximation we are making, are typically of the form

$$\left\langle\Phi\left|O_l\frac{1}{E^{(+)}-H_l}Q_l\right|\chi\right\rangle=\int_0^\infty\int_0^\infty\int_0^\infty\Phi^*(q)O_l(q,q')\frac{1}{k^2-q'^2}Q_l(q',q'')\chi(q'')dq\,dq'dq''$$
$$+\sum_{s=1}^{N_l}\sum_{s'=1}^{N_l}\left\{\int_0^\infty\int_0^\infty\Phi^*(q)O_l(q,q')\frac{1}{k^2-q'^2}f_s^{(l)}(q')dq\,dq'[\underline{A}_l^{(+)}(k)]_{ss'}^{-1}\right.$$
$$\left.\times\int_0^\infty\int_0^\infty f_{s'}^{(l)*}(q')\frac{1}{k^2-q'^2}Q_l(q',q'')\chi(q'')dq'dq''\right\}\ . \tag{4.1}$$

The operators $O_l(q,q')$ and $Q_l(q,q')$ and the functions $\Phi(q)$ and $\chi(q)$ are functions of the real momentum variables q and q', and they may also be functions of the wave number k, in which case, we shall assume that they may be analytically continued in this variable to the lower half plane. In general, the second term on the right-hand side of Eq. (4.1) has a pole at $k=k_n$ where the resolvent has a pole, while the first term is regular at k_n. The residue of the matrix element of the resolvent at the pole k_n may be evaluated with the help of (3.41) and (3.30):

$$\lim_{E\to E_n}(E-E_n)\left\langle\Phi\left|O_l\frac{1}{E^{(+)}-H_l}Q_l\right|\chi\right\rangle=\frac{\left[\int_0^\infty\Phi^*(q)O_l(q,q')u_{nl}(q')dq\,dq'\right]_{k_n}\left[\int_0^\infty u_{nl}(q)Q_l(q,q')\chi(q')dq\,dq'\right]_{k_n}}{\left[\int_0^\infty u_{nl}(q)dq\right]_{k_n}}\ . \tag{4.2}$$

This result shows that the matrix elements of quantum mechanical operators between properly normalized resonant states and an arbitrary state are given by

$$\langle\Phi\,|\,O_l\,|\,u_{nl}\rangle=\frac{\left[\int_0^\infty\Phi^*(q)O_l(q,q')u_{nl}(q';k)dq\,dq'\right]_{k_n}}{\left[\int_0^\infty u_{nl}^2(q;k)dq\right]_{k_n}^{1/2}} \tag{4.3}$$

and

$$\langle u_{nl}\,|\,Q_l\,|\,\chi\rangle=\frac{\left[\int_0^\infty u_{nl}(q;k)Q_l(q,q')\chi(q')dq\,dq'\right]_{k_n}}{\left[\int_0^\infty u_{nl}^2(q;k)dq\right]_{k_n}^{1/2}}\ . \tag{4.4}$$

The integrals are evaluated with $\mathrm{Im}k>0$, and then they are analytically continued to k_n.

It follows from this result that the normalization rule appropriate for resonant states in momentum representation is

$$\left[\int_0^\infty u_{nl}^2(q;k)dq\right]_{k_n}=1\ . \tag{4.5}$$

This rule simplifies the orthogonality condition (3.33) and makes the set of bound and resonant states an orthonormal set. It has the additional advantage of simplifying the relation between Gamow states and the resolvent of H_l.

We observe that when the left-hand side state of a matrix element is a resonant state, (4.4) requires that we use $u_{nl}(q;k)$ in the integral rather than its complex conjugate, as is usually required. This is a consequence of the non-self-adjoint character of the integral equation satisfied by resonant states. The corresponding problem in position representation of a Schrödinger equation with non-self-adjoint boundary conditions was discussed by Hokkyo[14] in the case of local short ranged potentials. In this same case, the rules for calculating matrix elements of operators between resonant states and for normalizing resonant states in position representation were obtained by Hokkyo,[14] García-Calderón, Peierls,[17] and Romo.[15] This last author also discussed the validity of the analytical continuation of the integrals in the k plane.

In what follows it will be shown that the norm of resonant states and the matrix elements between resonant states and arbitrary square integrable states are independent of the representation. It will be explicitly shown that, in the case of local short ranged potentials, the normalization rule derived in this work, Eq. (4.5), is equivalent to the prescription given by Hokkyo.[14]

First, we will show that resonant states in momentum representation $u_{nl}(q;k)$ are square integrable functions. From (3.20), (3.12), and (3.23) we obtain

$$\int_0^\infty u_{nl}^*(q;k)u_{nl}(q;k)dq=\frac{1}{k^2-k^{*2}}\sum_{\substack{s=1\\ s'=1}}^{N_l}\sum_{\substack{s''=1\\ s'''=1}}\{n_{nls}^*(k)v_{ss'}[G_{0ls's''}^{(+)}(k^*)-G_{0ls''s'}^{(+)}(k)]v_{s''s'''}n_{nls'''}(k)\} . \tag{4.6}$$

Let us call $(k^2-k^{*2})\underline{W}_l(k)$ the anti-Hermitian part of $\underline{G}_{0l}^{(+)}(k^*)$; in terms of $\underline{W}_l(k)$, Eq. (4.6) may be written as

$$\int_0^\infty u_{nl}^*(q;k)u_{nl}(q;k)dq=\underline{n}_{nl}^\dagger(k)\underline{v}\,\underline{W}_l(k)\underline{v}\,\underline{n}_{nl}(k) . \tag{4.7}$$

Since the right-hand side of (4.7) is the product of finite vectors and matrices and $\underline{W}_l$ is Hermitian when $\mathrm{Im}k>0$ and $\mathrm{Re}k>0$, the integral is finite and positive definite. Therefore, $u_{nl}(q;k)$ is square integrable and it has a Fourier transform

$$\hat{u}_{nl}(r;k)=\sqrt{2/\pi}\int_0^\infty \tilde{j}_l(qr)u_{nl}(q;k)dq . \tag{4.8}$$

The integral is defined with $\mathrm{Im}k>0$, and $\tilde{j}_l(x)$ is the Bessel-Riccati function of order l. The inverse relation is

$$u_{nl}(q;k)=\sqrt{2/\pi}\int_0^\infty \tilde{j}_l(qr)\hat{u}_{nl}(r;k)dr . \tag{4.9}$$

Similar relations are valid for $\chi_l(q)$ and $\Phi_l(q)$. Next, we insert these expressions in the integrals that appear in (4.3) and (4.4) and rearrange the integrals to obtain

$$\left[\int_0^\infty\int_0^\infty \Phi_l^*(q)O_l(q,q')u_{nl}(q';k)dq\,dq'\right]_{k_n}=\left[\int_0^\infty\int_0^\infty \hat{\Phi}_l^*(r)\hat{O}_l(r,r')\hat{u}_{nl}(r')dr\,dr'\right]_{k_n} , \tag{4.10}$$

where

$$\hat{O}_l(r,r')=\frac{2}{\pi}\int_0^\infty\int_0^\infty \tilde{j}_l(qr)O_l(q,q')\tilde{j}_l(q'r')dq\,dq' \tag{4.11}$$

and

$$\left[\int_0^\infty\int_0^\infty u_{nl}(q;k)Q_l(q,q')\chi_l(q')dq\,dq'\right]_{k_n}=\left[\int_0^\infty\int_0^\infty \hat{u}_{nl}(r;k)\hat{Q}_l(r;r')\hat{\chi}_l(r')dr\,dr'\right]_{k_n} . \tag{4.12}$$

$\hat{Q}_l(r,r')$ is related to $Q_l(q,q')$ by an expression similar to (4.11). Now, we insert (4.9) into the normalization integral and make use of the orthogonality of the Bessel-Riccati functions to obtain

$$\left[\int_0^\infty u_{nl}^2(q;k)dq\right]_{k_n}=\left[\int_0^\infty \hat{u}_{nl}^2(r;k)dr\right]_{k_n} . \tag{4.13}$$

Therefore, the normalization of resonant states and the matrix elements of quantum mechanical operators between resonant states and arbitrary states are independent of the representation.

When $\hat{u}_{nl}(r;k_n)$ is the solution of a radial Schrödinger equation with a cutoff potential of range R_0 and purely outgoing wave boundary conditions, $\hat{u}_{nl}(r,k_n)$ is equal to its asymptotic form $\hat{u}_{nl}^{(\mathrm{as})}(r;k_n)$ for $r>R_0$. For $l=0$,

$$\hat{u}_{n0}^{(\mathrm{as})}(r;k_n)=C_{n0}e^{ik_nr},\quad r>R_0 . \tag{4.14}$$

Then

$$\left[\int_0^\infty \hat{u}_{n0}^2(r;k)dr\right]_{k_n}=\left[\int_0^R \hat{u}_{n0}^2(r;k)dr+\left.\frac{\hat{u}_{n0}^{(\mathrm{as})^2}(r;k)}{2ik}\right|_R^\infty\right]_{k_n}$$

for $R>R_0$. Since $\mathrm{Im}k>0$, $\hat{u}_{n0}^{(\mathrm{as})}(r;k)$ vanishes when r goes to infinity, and the second term on the right-hand side gives a contribution only for $r=R$. Since the integral on the right-hand side is defined over a finite interval and $\hat{u}_{n0}(r;k)$ is an analytic function of k, we may take k_n inside the integration sign. In this way we arrive at the result

$$\left[\int_0^\infty u_{n0}^2(q;k)dq\right]_{k_n}=\int_0^R \hat{u}_{n0}^2(r;k_n)dr+i\frac{\hat{u}_{n0}^{(\mathrm{as})^2}(R;k_n)}{2k_n} \tag{4.15}$$

for any R larger than R_0. The right-hand side of equation (4.15) is the normalization condition for Gamow functions given by Hokkyo.[14]

It has already been shown that the integral of the modulus squared of $u_{nl}(q;k_n)$ exists, Eq. (4.7); this result suggests the possibility of normalizing Gamow states in momentum representation in terms of the integral of the square of the modulus of the wave function. Speaking in terms of physics, this makes sense since $u_{nl}(q;k_n)$ may be expanded as a linear superposition of scattering states of real energy, and $u_{nl}(q;k_n)$ may be interpreted as a wave packet. Therefore, we may calculate the expectation value of an operator according to the usual rule

$$\langle O_l\rangle''=\frac{\int_0^\infty\int_0^\infty u_{nl}^*(q;k_n)O_l(q,q')u_{nl}(q',k_n)dq\,dq'}{\int_0^\infty |u_{nl}(q;k_n)|^2dq} . \tag{4.16}$$

However, it will be shown that the result obtained according to (4.16) is not the expectation value of the operator $O_l(q,q')$ when the system is in a Gamow state, that is, in a purely outgoing particle state.

Since the wave packet $u_{nl}(q;k_n)$ is square integrable, it has a Fourier transform, but since $\mathrm{Re}k_n>0$ and $\mathrm{Im}k_n<0$, $u_{nl}(q;k_n)$ as a function of q has poles in the second and fourth quadrants. Its Fourier transform may be obtained from (2.11):

$$\sqrt{2/\pi}\int_0^\infty \tilde{j}_l(qr)u_{nl}(q;k_n)dq=-\frac{1}{k}\left[\tilde{j}_l(k_nr)\int_r^\infty h_l^{(-)}(k_nr')M_{nl}(r';k_n)dr'+h_l^{(-)}(k_nr)\int_0^r\tilde{j}_l(k_nr')M_{nl}(r';k_n)dr'\right]. \quad (4.17)$$

Therefore,

$$\sqrt{2/\pi}\int_0^\infty \tilde{j}_l(qr)u_{nl}(q;k_n)dq \underset{r\to\infty}{\longrightarrow} C_{nl}h_l^{(-)}(k_nr).$$

It follows that, although $u_{nl}(q;k_n)$ is the solution of the Lippmann-Schwinger equation (2.11) and, in this sense, we may call it the Gamow state wave function in momentum representation, the result obtained in (4.16) is the expectation value of the operator O_l when the system is in a purely incoming particle state. This seemingly paradoxical result is owing to the fact that, in momentum representation, the functional dependence of the Gamow state wave function $u_{nl}(q;k)$ on k carries two different pieces of information that depend on the location of k in the complex plane. In the first place, the fact that $u_{nl}(q;k_n)$ is a solution of the homogeneous Lippmann-Schwinger equation for outgoing particles that belong to the complex energy eigenvalue E_n requires that $k=k_n$, with $\mathrm{Re}k_n>0$ and $\mathrm{Im}k_n<0$. Second, the location of the two poles of $u_{nl}(q;k)$ coming from the energy denominator in (2.11) in the first and third quadrants of the q plane determines the purely outgoing nature of the state, that is, $u_{nl}(q;k)$ represents a purely outgoing particle state when $\mathrm{Re}k>0$ and $\mathrm{Im}k>0$. It is clear now that, in order to keep all this information, the integrals occurring in the calculation of matrix elements and the normalization integral must first be defined correctly with k in the upper half of the k plane. Only after the integrals have been correctly defined may they be analytically continued to k_n in the fourth quadrant of the k plane to obtain the matrix elements of operators defined between purely outgoing particle states of complex momentum k_n, as is done in Eqs. (4.3) and (4.4).

We have still to examine another possibility of defining a norm of $u_{nl}(q;k_n)$ in terms of its modulus squared. The expansion

$$u_{nl}(q;k_n)=\sum_{s=1}^{\infty}n_{nls}(k_n)f_s^{(l)}(q) \quad (4.18)$$

suggests the definition

$$(u_{nl}\,|\,u_{nl})=\sum_{s=1}^{\infty}|n_{nls}(k_n)|^2. \quad (4.19)$$

We use parentheses to avoid any confusion with our previous results. From (3.8)

$$(u_{nl}\,|\,u_{nl})=\left[\sum_{s=1}^{\infty}|n_{nl}(k)|^2\right]_{k_n}$$

$$=\left[\int_0^\infty |u_{nl}(q;k)|^2dq\right]_{k_n}. \quad (4.20)$$

As in previous expressions, the integral is defined with $\mathrm{Im}k>0$ and then is continued to k_n.

Now, it may be shown that the term on the right-hand side of Eq. (4.20) vanishes identically. In order to do this let us consider the Schrödinger equation for $u_{nl}(q;k_n)$ in momentum representation:

$$(k_n^2-q^2)u_{nl}(q;k_n)-\left[\int_0^\infty U_l(q,q')u_{nl}(q';k)dq\right]_{k_n}=0. \quad (4.21)$$

As explained in Sec. II, the notation means that the integral in square brackets is defined with k in the upper half of the wave number plane, and the resulting function of k is analytically continued to k_n in the lower half of that plane. When the left-hand side of Eq. (4.21) is evaluated at k rather than k_n, the right-hand side of the equation is no longer zero, but we may always write

$$(k^2-q^2)u_{nl}(q;k)-\int_0^\infty U_l(q,q')u_{nl}(q';k)dq'=(k^2-k_n^2)g(q;k), \quad (4.22)$$

with $\mathrm{Im}k>0$. From (4.21) and (4.22), it follows that

$$g(q;k_n)=\left\{\frac{\partial}{\partial k^2}\left[(k^2-q^2)u_{nl}(q;k)-\int_0^\infty U_l(q,q')u_{nl}(q';k)dq'\right]\right\}_{k_n}, \quad (4.23)$$

which, in general, is not zero.

Now, we take the complex conjugate of Eq. (4.22),

$$(k^{*2}-q^2)u_{nl}^*(q;k)-\int_0^\infty U_l(q,q')u_{nl}^*(q';k)dq'=(k^{*2}-k_n^{*2})g^*(q;k). \quad (4.24)$$

Next, we multiply (4.22) and (4.24) by $u_{nl}(q;k)$ and $u_{nl}^*(q;k)$, respectively, integrate over q, and take the difference; in this way we obtain

$$(k^2-k^{*2})\int_0^\infty |u_{nl}(q;k)|^2dq=(k^2-k_n^2)\int_0^\infty g(q;k)u_{nl}^*(q;k)dq-(k^2-k_n^2)^*\int_0^\infty g^*(q;k)u_{nl}(q;k)dq\ . \tag{4.25}$$

All the integrals in (4.25) are defined with $\mathrm{Im}k>0$. We take the limit when k goes to k_n on both sides of Eq. (4.25) and, recalling that $\mathrm{Im}k_n^2=-i(m/\hbar^2)\Gamma_n$, we obtain

$$\frac{2m}{\hbar^2}\Gamma_n\left[\int_0^\infty |u_{nl}(q;k)|^2dq\right]_{k_n}=0\ . \tag{4.26}$$

Since the resonance width $\Gamma_n\neq 0$, it follows that

$$\left[\int_0^\infty |u_{nl}(q;k)|^2dq\right]_{k_n}=0\ . \tag{4.27}$$

From this result it follows that, when $\Gamma_n\neq 0$, a resonant state in momentum representation cannot be normalized in terms of its modulus defined as in (4.19), since the integral in (4.20) vanishes at k_n.

V. EXPANSIONS IN TERMS OF A SET OF BOUND, RESONANT AND SCATTERING STATES

In this section it will be shown that an arbitrary square integrable state in momentum space representation may be expanded in terms of a set containing bound and resonant states, and a continuum of scattering wave functions of complex wave number. The expansion coefficients are expressed as integrals of well-behaved functions.

We start by recalling that the orthonormal set of bound and scattering solutions of the Schrödinger equation form a complete set. This has been shown for local[21] and nonlocal[31] potentials under fairly general conditions. Then, for any two square integrable functions $\Phi(q)$ and $X(q)$, the following relation holds:

$$\int_0^\infty \Phi^*(q)X(q)dq=\sum_{\substack{m\\ \text{(bound states)}}}\langle\Phi|u_{ml}\rangle\langle u_{ml}|X\rangle+\int_0^\infty\langle\Phi|u_{kl}\rangle\langle u_{kl}|X\rangle dk\ , \tag{5.1}$$

where

$$\langle\Phi|u_{ml}\rangle=\int_0^\infty\Phi^*(q)u_{ml}(q)dq\ ,\qquad \langle u_{ml}|X\rangle=\int_0^\infty u_{ml}^*(q)X(q)dq\ , \tag{5.2}$$

and

$$\langle\Phi|u_{kl}\rangle=\int_0^\infty\Phi^*(q)u_{kl}(q)dq\ ,\qquad \langle u_{kl}|X\rangle=\int_0^\infty u_{kl}^*(q)X(q)dq\ . \tag{5.3}$$

The partial wave function $u_{ml}(q)$ is a bound state solution of the homogeneous Lippmann-Schwinger equation (3.7) (3.8), corresponding to a negative energy E_m, and $u_{kl}(q)$ is a scattering partial wave function which satisfies the inhomogeneous Lippmann-Schwinger equation

$$u_{kl}(q)=\delta(q-k)+\int_0^\infty\int_0^\infty\frac{\delta(q-q')}{k^{2(+)}-q'^2}U_l^{(N_l)}(q',q'')\times u_{kl}(q'')dq'dq''\ . \tag{5.4}$$

The explicit form of the solution of (5.4) is

$$u_{kl}(q)=\sum_{s=1}^{N_l}\sum_{s'=1}^{N_l}f_s^{(l)}(q)\left[\delta_{ss'}+(A_l^{(+)}(k))_{ss'}^{-1}\frac{1}{k^2-q^2}\right]f_{s'}^{(l)*}(k)\ . \tag{5.5}$$

In general, the functions $\Phi(q)$ and $X(q)$ are functions of the real momentum q, and they may also be functions of the wave number (energy) k. In this case we will assume that, as functions of k, they may be analytically continued to the lower half of the k plane. Then, from (5.3) and (5.5), it follows that the term $\langle\Phi|u_{kl}\rangle\langle u_{kl}|X\rangle$ may also be analytically continued to the lower half of the k plane.

Now, from the spectral representation of the resolvent of H_l for outgoing (incoming) particles,

$$\left\langle q\left|\frac{1}{E^{(\pm)}-H_l}\right|q'\right\rangle=\sum_m u_{ml}(q)\frac{1}{E-E_m}u_{ml}^*(q')+\int_0^\infty u_{k'l}^*(q)\frac{1}{k^{2(\pm)}-k'^2}u_{k'l}(q')dk'\ , \tag{5.6}$$

with $k^{2(\pm)}$ in the upper (lower) half of the k plane, and from the Plemelj formulae,[24] it follows that

$$2\pi i\langle\Phi|u_{kl}\rangle\langle u_{kl}|X\rangle=\int_0^\infty\int_0^\infty\Phi^*(q)\left[\left\langle q\left|\frac{1}{k^{2(+)}-H_l}\right|q'\right\rangle-\left\langle q\left|\frac{1}{k^{2(-)}-H_l}\right|q'\right\rangle\right]X(q')dq\,dq'\ . \tag{5.7}$$

The resolvent for incoming particles that appears in (5.7), as a function of k, may be analytically continued to the lower half of the k plane without crossing the real axis, and it has no singularities in that part of the plane. The analytic continuation of the resolvent for outgoing particles may have poles in the lower half of the k plane. Now, the integration contour of Eq. (5.1) is deformed into the lower half plane, as shown in Fig. 1. When the deformed contour C crosses over resonant poles, but avoids other singularities of the analytically continued integrand, the theorem of the residue yields

$$2\pi i\langle\Phi\,|\,u_{kl}\rangle\langle u_{kl}\,|\,\chi\rangle=\sum_{\substack{n\\ \text{(resonant states)}}}\text{res}\left\{\left[\int_0^\infty\int_0^\infty\Phi^*(q)\left\langle q\left|\frac{1}{k^{2(+)}-H_l}\right|q'\right\rangle\chi(q')dq\,dq'\right]_{k_n}\right\}$$
$$+\int_C dz\left[\int_0^\infty\Phi^*(q)u_{kl}(q)dq\int_0^\infty\tilde{u}_{kl}(q')\chi(q')dq'\right]_{k=Z}, \tag{5.8}$$

with $z=2^{-1/2}(1-i)k$. Right and left eigenvectors are distinguished with a tilde on the left eigenvector. This distinction is made because when the wave number is complex, the left eigenvectors are not equal to the Hermitian conjugate of the right eigenvectors. It was shown in Sec. III that, in the case of spinless particles, $\langle\tilde{u}_{nl}\,|\,q\rangle=\langle q\,|\,u_{nl}\rangle=u_{nl}(q)$.

Since $\Phi(q)$ and $\chi(q)$ are arbitrary, the above discussion justifies writing the expansion

$$\chi(q)=\sum_{\substack{m\\ \text{(bound states)}}}u_{ml}(q)\langle u_{ml}\,|\,\chi\rangle+\sum_{\substack{n\\ \text{(resonant states)}}}u_{nl}(q)\langle\tilde{u}_{nl}\,|\,\chi\rangle+\int_C u_{zl}(q)\langle\tilde{u}_{zl}\,|\,\chi\rangle dz\,. \tag{5.9}$$

The expansion coefficients are given by

$$\langle u_{ml}\,|\,\chi\rangle=\int_0^\infty u_{ml}(q)\chi(q)dq\,, \tag{5.10}$$

$$\langle\tilde{u}_{nl}\,|\,\chi\rangle=\left[\int_0^\infty u_{nl}(q;k)\chi(q)dq\right]_{k_n}, \tag{5.11}$$

$$\langle\tilde{u}_{zl}\,|\,\chi\rangle=\left[\int_0^\infty u_{kl}(q)\chi(q)dq\right]_{k=z}. \tag{5.12}$$

Matrix elements of the resolvent operator of H_l for outgoing particles may also be expressed as a summation over bound and resonant states, and an integral over a continuum of scattering functions. This result follows immediately from the spectral representation of the resolvent operator, Eq. (5.6), defined with k in the upper half plane, when this resolvent, as a function of the wave number k, is analytically continued to the lower half of the k plane and the integration contour that appears in (5.6) is deformed as explained in the preceding discussion. In this way, we obtain the following expansion:

$$\left\langle\Phi\left|\frac{1}{k^{2(+)}-H_l}\right|\chi\right\rangle=\sum_{\substack{m\\ \text{(bound states)}}}\langle\Phi\,|\,u_{ml}\rangle\frac{1}{k^2-k_m^2}\langle u_{ml}\,|\,\chi\rangle+\sum_{\substack{n\\ \text{(resonant states)}}}\langle\phi\,|\,u_{nl}\rangle\frac{1}{k^2-k_n^2}\langle\tilde{u}_{nl}\,|\,\chi\rangle$$
$$+\int_C\langle\Phi\,|\,u_{zl}\rangle\frac{1}{k^2-z^2}\langle\tilde{u}_{zl}\,|\,\chi\rangle dz\,. \tag{5.13}$$

The expansion coefficients are given in (5.11), (5.12), and (5.10), and

$$\langle\Phi\,|\,u_{ml}\rangle=\int_0^\infty\Phi^*(q)u_{ml}(q)dq\,, \tag{5.14}$$

$$\langle\Phi\,|\,u_{nl}\rangle=\left[\int_0^\infty\Phi^*(q)u_{nl}(q;k^{(+)})dq\right]_{k_n}, \tag{5.15}$$

$$\langle\Phi\,|\,u_{zl}\rangle=\left[\int_0^\infty\Phi^*(q)u_{kl}(q)dq\right]_{k=z}. \tag{5.16}$$

Again, since $\Phi(q)$ and $\chi(q)$ are arbitrary functions, we are justified in writing the expansion

$$\left\langle q\left|\frac{1}{k^{2(+)}-H_l}\right|q'\right\rangle=\sum_{\substack{m\\ \text{(bound states)}}}u_{ml}(q)\frac{1}{k^2-k_m^2}u_{ml}(q')+\sum_{\substack{n\\ \text{(resonant states)}}}u_{nl}(q;k_n)\frac{1}{k^2-k_n^2}u_{nl}(q';k_n)$$
$$+\int_C u_{zl}(q)\frac{1}{k^2-z^2}\tilde{u}_{zl}(q')dz\,. \tag{5.17}$$

It must be kept in mind that, when using these expansions for the calculation of transition amplitudes or matrix elements, one must be careful to define the integrals of resonant and scattering states appearing in (5.17) with the wave numbers in the upper half plane and then continue them analytically to k_n or z in the lower half plane in order to obtain physically and mathematically sound results.

VI. GAMOW STATES OF A DELTA SHELL POTENTIAL IN THE MOMENTUM REPRESENTATION

The properties of resonant states in momentum representation discussed previously are illustrated with a simple example. These results are compared with the well-known properties of Gamow functions of local short ranged potentials in position representation. The so-called delta

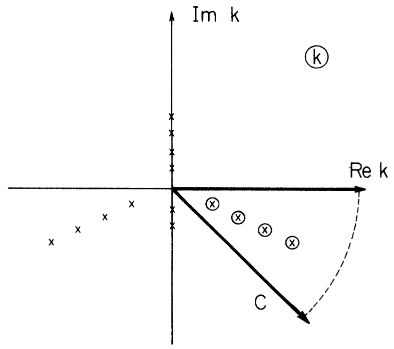

FIG. 1. The straight line with slope -1 is the integration contour C in the wave number plane k that appears in Eqs. (5.10) and (5.14). The dashed line shows the way in which the original contour along the positive real axis is deformed into the lower half of the plane, passing over the proper resonant poles (circles) to obtain the new contour.

shell potential is particularly well suited for this purpose, since it is local and short ranged in position representation, while it is separable of rank one in momentum representation.

In position representation, the delta shell potential is defined as

$$\langle r \mid V \mid r' \rangle = \frac{\hbar^2}{2ma}\lambda\delta(r-a)\delta^{(3)}(\vec{r}-\vec{r}\,') . \quad (6.1)$$

The momentum representation of the potential (6.1) is

$$\langle p \mid V \mid p' \rangle = \frac{\hbar}{\pi m a}\lambda \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\hat{p})\frac{\tilde{j}_l(p/\hbar a)}{p}\frac{\tilde{j}_l(p'/\hbar a)}{p'} \times Y_{lm}^{*}(\hat{p}\,') , \quad (6.2)$$

where $\tilde{j}_l(x)$ is the Riccati-Bessel function of order l.

In this case, the Lippmann-Schwinger equation (2.11) for the partial wave $u_{nl}(p)$ is

$$u_{nl}(q;k_n) = \frac{2}{\pi a}\lambda\left[\int_0^{\infty}\frac{\delta(q-q')}{k^{2(+)}-q'^2}\tilde{j}_l(q'a)dq' \times \int_0^{\infty}\tilde{j}_l(q''a)u_{nl}(q'',k)dq''\right]_{k_n} . \quad (6.3)$$

We recall that $\hbar q = p$.

In what follows we will solve (6.3) in the particular case of $l=0$:

$$u_{n0}(q;k_n) = \frac{2\lambda}{\pi a}\left[\int_0^{\infty}\frac{\delta(q-q')}{k^2-q'^2}\sin q'a\, dq'\right]_{k_n} \times \left[\int_0^{\infty}\sin q''a u_{n0}(q'',k)dq''\right]_{k_n} . \quad (6.4)$$

We seek a function $u_{n0}(q;k)$, of the real variable q and the complex variable k, such that it satisfies (6.4) when the integral on the right-hand side of this equation is defined with k in the upper half of the k plane and then it is analytically continued to k_n in the lower half of that plane.

The existence condition for solutions of (6.4) is the vanishing of the Fredholm determinant, which, in this case, is given by

$$\Delta_0^{(+)}(k) = 1 - \frac{2\lambda}{\pi a}\int_0^{\infty}\frac{\sin^2 qa}{k^2-q^2}dq . \quad (6.5)$$

The integral in (6.5) is also defined with k in the upper half of the k plane. The integration is readily performed to yield

$$\Delta_0^{(+)}(k) = 1 + \frac{\lambda}{ka}e^{ika}\sin ka . \quad (6.6)$$

Therefore, the integral equation (6.4) has an infinite number of solutions of the form

$$u_{n0}(q;k_n) = \sqrt{2/\pi}\frac{\lambda}{a}n_n(k_n)\frac{1}{k_n^2-q^2}\sin qa , \quad (6.7)$$

where k_n is a root of the transcendental equation

$$1 + \frac{\lambda}{k_n a}e^{ik_n a}\sin k_n a = 0 . \quad (6.8)$$

Multiplying both sides of (6.8) by $e^{-ik_n a}$ and writing the exponential in terms of trigonometric functions, the existence condition (6.8) may also be written as

$$\sin k_n a\left[\frac{\lambda}{k_n a} - i\right] + \cos k_n a = 0 .$$

Writing

$$k_n = \kappa_n - i\gamma_n ,$$

with κ_n and γ_n real, and separating real and imaginary parts in (6.8), we obtain the set of coupled equations

$$\frac{2\gamma_n a}{\lambda} + e^{2\gamma_n a}\cos 2\kappa_n a - 1 = 0 \quad (6.9)$$

and

$$\frac{2\kappa_n a}{\lambda} + e^{2\gamma_n a}\sin 2\kappa_n a = 0 . \quad (6.10)$$

When λ is positive, the solutions of (6.9) and (6.10) are of the form

$$\kappa_n = \frac{1}{a}\left[\frac{4n-1}{4}\pi + \delta_n(\lambda)\right] \quad (6.11)$$

and

$$\gamma_n = \frac{1}{2a}\left\{\lambda - \left[\frac{4n-1}{2}\pi + 2\delta_n(\lambda)\right]\tan 2\delta_n(\lambda)\right\} , \quad (6.12)$$

with $n = 1,2,3,4,\ldots$, and

$$0 \le \delta_n(\lambda) \le \frac{\pi}{2} .$$

The resonant state $u_{n0}(p;k_n)$ is normalized according to (6.11)

$$\left[\int_0^\infty u_{n0}^2(p;k)dp\right]_{k_n}=1 . \tag{6.13}$$

Substitution of (6.7) in (6.13) yields

$$\frac{2}{\pi}\left[\frac{\lambda}{a}\right]^2 n_n^2\left[\int_0^\infty \frac{\sin^2 qa}{(k^2-q^2)^2}dq\right]_{k_n}=1 . \tag{6.14}$$

The integration is readily performed, and we obtain

$$\int_0^\infty \frac{\sin^2 qa}{(k^2-q^2)^2}dq=\frac{\pi}{4k^3}\sin ka\, e^{ika}[-1+ika+ka\cot ka] .$$

Evaluating this function in $k=k_n$ and simplifying with the help of the existence condition (6.8),

$$\left[\int_0^\infty \frac{\sin^2 qa}{(k^2-q^2)^2}dq\right]_{k_n}=\frac{k_n a}{\lambda}[1+\lambda-i2k_n a] . \tag{6.15}$$

Inserting this result in the normalization condition (6.3) yields the normalization constant

$$n_n(k_n)=k_n\left[\frac{2a}{\hbar\lambda(1+\lambda-i2k_n a)}\right]^{1/2} . \tag{6.16}$$

Hence, the normalized Gamow state is

$$u_{n0}(q;k_n)=\sqrt{2/\pi\hbar}\left[\frac{2\lambda}{a(1+\lambda-2ik_n a)}\right]^{1/2} \times\frac{k_n}{k_n^2-q^2}\sin qa . \tag{6.17}$$

In Sec. IV, it was shown that the integral of the modulus squared of the Gamow function $u_{n0}(q;k)$ defined with k in the upper half of the k plane vanishes when evaluated in k_n. This result is easily verified in the example at hand:

$$\int_0^\infty |u_{n0}(q;k)|^2 dq =|n_n|^2\frac{2}{\pi}\left[\frac{\lambda}{a}\right]^2\hbar\int_0^\infty \frac{\sin^2 qa}{|k^2-q^2|^2}dq , \tag{6.18}$$

with $\mathrm{Im}k>0$. The integration is easily performed writing $\sin^2 qa$ in terms of exponentials and using Cauchy's theorem. In this way we obtain

$$\int_0^\infty |u_{n0}(q;k)|^2 dq=|n_n|^2\frac{2}{\pi}\left[\frac{\lambda}{a}\right]^2\frac{\pi}{4(k-k^*)(k+k^*)}\frac{1}{|k|^2}\{i(k+k^*)-i(k^* e^{2ika}+ke^{-2ik^*a})\} , \tag{6.19}$$

which can be written in terms of κ_n and γ_n as

$$\left[\int_0^\infty |u_{n0}(q;k)|^2 dq\right]_{k_n}=\frac{|n_n|^2}{2\gamma_n}\frac{\lambda^2\hbar}{|k_n a|^2}\left\{e^{2\gamma_n a}\left[\cos\kappa_n a-\frac{\gamma_n}{\kappa_n}\sin 2\kappa_n a\right]-1\right\} . \tag{6.20}$$

Making use of (6.9) and (6.10), we finally get

$$\left[\int_0^\infty |u_{n0}(q;k)|^2 dq\right]_{k_n}=0 . \tag{6.21}$$

In Sec. IV, it was shown that the residue of the resolvent of H_l, in a simple pole, is equal to $u_{nl}^2(q;k_n)$ when the Gamow functions are normalized to one. This relation is readily verified in this example. The integral equation for the resolvent

$$\left\langle p\left|\frac{1}{E^{(+)}-H_0}\right|p'\right\rangle=\frac{\delta(p-p')}{E-\frac{p^2}{2m}}+\frac{\hbar\lambda}{\pi ma}\int_0^\infty dp''\int_0^\infty dp'''\left[\frac{\delta(p-p'')}{E-\frac{p'^2}{2m}}\sin\left[\frac{p''a}{\hbar}\right]\sin\left[\frac{p'''a}{\hbar}\right]\left\langle p'''\left|\frac{1}{E-H_0}\right|p'\right\rangle\right] \tag{6.22}$$

is solved to give

$$\left\langle p\left|\frac{1}{E-H_0}\right|p'\right\rangle=\frac{\delta(p-p')}{E-\frac{p^2}{2m}}+\frac{\hbar\lambda}{\pi ma}\frac{\sin qa}{E-\frac{p^2}{2m}}\frac{1}{1+\frac{\lambda}{ka}e^{ika}\sin ka}\frac{\sin q'a}{E-\frac{p'^2}{2m}} . \tag{6.23}$$

When E_n is a simple pole,

$$\lim_{E\to E_n}(E-E_n)\left\langle p\left|\frac{1}{E-H_0}\right|p'\right\rangle=\frac{\hbar^2\lambda}{\pi ma}\frac{\sin qa}{E_n-\frac{p^2}{2m}}\frac{1}{\left[\frac{d}{dE}\left[1+\frac{\lambda}{ka}e^{ika}\sin ka\right]\right]_{k_n}}\frac{\sin q'a}{E_n-\frac{p^2}{2m}} . \tag{6.24}$$

Now

$$\frac{d}{dE}\left[1+\frac{\lambda}{ka}e^{ika}\sin ka\right]_{k_n}=\frac{\hbar^2}{2m}\frac{\lambda}{2k_n^3 a}[k_n a\cot k_n a+ik_n a-1]e^{ik_n a}\sin k_n a .$$

This expression may be simplified with the help of (6.8) and (6.9):

$$\left[\frac{d}{dE}\left[1+\frac{\lambda}{ka}e^{ika}\sin ka\right]\right]_{k_n}=\frac{\hbar^2}{2m}\frac{1}{2k_n}[1+\lambda-i\,2k_na]\;. \tag{6.25}$$

Substitution of (6.25) in (6.24) yields

$$\lim_{E\to E_n}(E-E_n)\left\langle p\left|\frac{1}{E-H_0}\right|p'\right\rangle=\left[\frac{4\lambda}{\pi\hbar a(1+\lambda-i\,2k_na)}\right]^{1/2}\frac{k_n}{k_n^2-q^2}\sin qa\left[\frac{4\lambda}{\pi\hbar a(1+\lambda-i\,2k_na)}\right]^{1/2}\frac{k_n}{k_n^2-q'^2}\sin q'a\;, \tag{6.26}$$

which is the product of two Gamow functions correctly normalized.

In position representation, the resonant states in a delta shell potential, with $l=0$, are the solutions of the radial equation

$$\frac{d^2\hat{u}_{n0}(r)}{dr^2}+k_n^2\hat{u}_{n0}(r)-\frac{\lambda}{a}\delta(r-a)\hat{u}_{n0}(r)=0\;, \tag{6.27}$$

which are regular at the origin and behave as pure outgoing waves for r larger than a. At $r=a$, the function $\hat{u}_{n0}(r)$ is continuous, but its derivative is discontinuous so as to satisfy (6.27),

$$\left.\frac{d\hat{u}_{n0}(r)}{dr}\right|_{a+}=\left.\frac{d\hat{u}_{n0}(r)}{dr}\right|_{a-}+\lambda\hat{u}_{n0}(a)\;. \tag{6.28}$$

A solution of (6.28) satisfying the boundary condition stated above and the continuity condition is

$$\begin{aligned}\hat{u}_{n0}(r)&=Ne^{ik_na}\sin k_nr,\quad 0\le r<a\\ &=N\sin k_nae^{ik_nr},\quad r>a\;.\end{aligned} \tag{6.29}$$

When the solution (6.29) is inserted in (6.28), we obtain the existence condition for solutions of (6.27),

$$\sin k_na[\lambda-ik_na]+k_na\cos k_na=0\;. \tag{6.30}$$

Combining the two terms proportional to k_na into one exponential function, it is verified that (6.30) is equivalent to

$$1+\frac{\lambda}{k_na}e^{ik_na}\sin k_na=0\;, \tag{6.31}$$

which is the existence condition for solutions of the integral equation (6.4).

The normalization condition for Gamow states according to Peierls[7] and Hokkyo[14] is

$$N_n^2\left[e^{2ik_na}\int_0^a\sin^2k_nr\,dr+i\frac{\sin^2k_nae^{i2k_na}}{2k_n}\right]=1\;.$$

This yields

$$N_n^2\left\{\frac{e^{i2k_na}}{2k_na}[k_na-\sin k_nae^{-ik_na}]\right\}=1\;.$$

Simplifying with the help of (6.30), we obtain

$$N_n=\left[\frac{2\lambda}{1+\lambda-i\,2k_na}\right]^{1/2}\;. \tag{6.32}$$

In Sec. IV, we found that resonant states in momentum representation are transformed to position representation according to

$$\hat{u}_{nl}(r;k_n)=\sqrt{2\hbar/\pi}\left[\int_0^\infty\tilde{j}_l(qr)u_{nl}(q;k)dq\right]_{k_n}\;.$$

In the example we are discussing, we must evaluate

$$\hat{u}_{n0}(r;k_n)=\left[\frac{2}{\pi}\right]\left[\frac{2\lambda}{a(1+\lambda-i\,2k_na)}\right]^{1/2}k_n\times\left[\int_0^\infty\frac{\sin qr\,\sin qa}{k^2-q^2}dq\right]_{k_n}\;.$$

The integration yields

$$\begin{aligned}\int_0^\infty\frac{\sin kr\,\sin qa}{k^2-q^2}dq&=\frac{\pi}{2k}\sin kae^{ikr},\quad r>a\\ &=\frac{\pi}{2k}e^{ika}\sin kr,\quad r<a\;,\end{aligned}$$

which, when substituted in the expression for $\hat{u}_{n0}(r;k_n)$, yields

$$\begin{aligned}\hat{u}_{n0}(r;k_n)&=\left[\frac{2\lambda}{a(1+\lambda-i\,2k_na)}\right]^{1/2}e^{ik_na}\sin k_nr,\quad r<a\\ &=\left[\frac{2\lambda}{a(1+\lambda)-i\,2k_na)}\right]^{1/2}\sin k_nae^{ik_nr},\quad r>a\;,\end{aligned}$$

in agreement with (6.29) and (6.32).

VII. SUMMARY

In this paper, Gamow states in momentum representation are defined as right solutions of a homogeneous Lippmann-Schwinger equation for purely outgoing particle states. This condition makes the problem non-self-adjoint. Therefore, resonant states are eigenfunctions of the Schrödinger equation in momentum representation belonging to complex energy eigenvalues with a negative imaginary part. Although there is no difficulty of principle in extending the theory to include the Coulomb interaction, in order to avoid unnecessary complications, it was not considered here.

The potential $U_l(q,q')$ was approximated by means of a separable potential of rank N_l, and the Lippmann-Schwinger equation was solved with this potential for N_l arbitrarily large. It was found that resonant states in momentum representation are square integrable functions.

This is in sharp contrast with the well-known properties of resonant states in position representation which are waves of exponentially increasing amplitude.

Some properties of resonant states in momentum representation are the following:

(i) The adjoint (left solution of the integral equation) of the Gamow state function is the same function rather than the complex conjugate.

(ii) The norm of a resonant state is the integral of the square of the Gamow function $u_{nl}(q;k)$, defined with k in the upper half of the wave number plane and then analytically continued to k_n in the lower half of the plane.

(iii) Bound and resonant states form a biorthonormal set with their adjoints.

(iv) Matrix elements of quantum mechanical operators between properly normalized resonant states and arbitrary states are obtained as integrals defined with the wave number $k=(2mE/\hbar^2)^{1/2}$ in the upper half of the k plane.

(v) The position representation of a Gamow state is obtained from its momentum representation as the Fourier transform of $u_{nl}(q;k)$ defined with $\mathrm{Im}k>0$, and then analytically continued to k_n. The momentum representation of a Gamow state is obtained from its position representation in a similar way.

(vi) The norm of a Gamow state is independent of the representation. In fact, with the help of (iv), it was shown that the norm of resonant states defined in this work is equal to the norm defined by Hokkyo[14] and Romo[15] in position representation.

It was also shown that, although Gamow state functions in momentum representation are square integrable, Gamow states are unnormalizable in terms of the integral of the modulus squared of the state function. It is possible to define a normalized momentum probability density in terms of $|u_{nl}(q;k_n)|^2$. However, since $\mathrm{Im}k_n<0$, the expectation values obtained with this probability density correspond to purely incoming particle states rather than to Gamow states. When we try to define the normalization integral in terms of

$$\int_0^\infty |u_{nl}(q;k)|^2 dq$$

with $\mathrm{Im}k>0$, it corresponds to outgoing particle states, but when the integral is analytically continued to the Gamow state wave number k_n, it vanishes. Therefore, when we try to calculate expectation values of quantum mechanical operators as the analytic continuation to k_n of the integral

$$\int_0^\infty \int_0^\infty u_{nl}^*(q;k)O_l(q,q')u_{nl}(q,k)dq\,dq'$$

defined with $\mathrm{Im}k>0$, the results are finite, but cannot be normalized.

Following a standard procedure, it was shown that a square integrable function may be expanded in terms of a set containing bound and resonant states, and a continuum of scattering functions of complex wave number.

Finally, to illustrate these results with an example, we discussed the properties of resonant states in a potential shell, both in momentum and in position representation.

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APPENDIX

It will be shown that:

(i) The location of the poles of the resolvent of $H_l^{(N_l)}$ and the collision matrix S_l in the wave number plane k is determined by the zeros of the determinant $\Delta_l^{(+)}(k)$ of $\underline{1}-\underline{K}_l^{(+)}(k)$.

(ii) The zeros of $\Delta_l^{(+)}(k)$ are located on the imaginary axis and in the lower half of the momentum plane k including the real axis.

The restriction of the resolvent of $H_l^{(N_l)}$ to the lth wave satisfies the integral equation

$$\left\langle q \left| \frac{1}{k^2+i\epsilon-H_l^{(N_l)}} \right| q' \right\rangle = \frac{\delta(q-q')}{k^2+i\epsilon-q^2} + \frac{1}{k^2+i\epsilon-q^2} \sum_{s=1}^{N_l} \sum_{s'=1}^{N_l} f_s^{(l)}(q) v_{ss'}^{(l)} \int_0^\infty f_{s'}^{(l)*}(q'') \left\langle q'' \left| \frac{1}{k^2+i\epsilon-H_l^{(N_l)}} \right| q' \right\rangle dq'' , \tag{A1}$$

which has the solution

$$\left\langle q \left| \frac{1}{k^2+i\epsilon-H_l^{(N_l)}} \right| q' \right\rangle = \frac{1}{k^2+i\epsilon-q'^2} + \frac{1}{k^2+i\epsilon-q^2} \sum_{s=1}^{N_l} \sum_{s'=1}^{N_l} f_s^{(l)}(q) (\underline{A}_l^{(+)}(k))_{ss'}^{-1} f_{s'}^{(l)*}(q') \frac{1}{k^2+i\epsilon-q'^2} , \tag{A2}$$

where

$$\underline{A}_l^{(+)}(k)=\underline{v}^{-1}-\underline{G}_{0l}^{(+)}(k)=(\underline{1}-\underline{K}_l^{(+)}(k))\underline{v}^{-1} .$$

The inverse of $\underline{A}_l^{(+)}(k)$ is

$$\underline{A}_l^{(+)}(k)^{-1}=\frac{\hat{\underline{A}}_l^{(+)}(k)}{\Delta_l^{(+)}(k)}\det\underline{v} . \tag{A3}$$

$\hat{\underline{A}}_l^{(+)}(k)$ is the arithmetic complement of $\underline{A}_l^{(+)}(k)$, and $\Delta_l^{(+)}(k)$ is the determinant of $\underline{1}-\underline{K}_l^{(+)}(k)$.

Once the resolvent (A2) is known, the S_l matrix is readily obtained

$$S_l=\mathrm{tr}\{\underline{A}_l^{(-)}(k)(\underline{A}_l^{(+)}(k))^{-1}\}-(N_l-1) . \tag{A4}$$

From Eqs. (3.12) and (3.13), the matrix elements $G^{(+)}_{0l,ss'}(k)$ are holomorphic functions of k for all finite values of k when the functions $f_s^{(l)}(q)$ are entire and Hölder continuous,[24] in this case $\underline{A}_l^{(+)}(k)$ and $\hat{\underline{A}}_l^{(+)}(k)$ are also holomorphic for all finite k. It follows from (A2), (A3), and (A4) that the poles of the S_l matrix and the resolvent

$$\left\langle q \left| \frac{1}{k^2 - H_l^{(N)}} \right| q' \right\rangle$$

in the wave number k plane are determined by the zeros of the determinant $\Delta_l^{(+)}(k)$.[21]

Now, since $\det(\underline{v}) \neq 0$, the condition

$$\Delta_l^{(+)}(k_n) = 0 \tag{A5}$$

is a necessary and sufficient condition for the existence of solutions of the homogeneous linear equations

$$\underline{G}_{0l}^{(+)}(k_n)\underline{m}_{nl} = \underline{v}^{-1}\underline{m}_{nl} \ . \tag{A6}$$

Taking the adjoint of this expression

$$\underline{m}_{nl}^{\dagger}\underline{G}_{0l}^{(+)\dagger}(k_n) = \underline{m}_{nl}^{\dagger}\underline{v}^{-1} \ . \tag{A7}$$

Multiplying (A7) on the right by $\underline{m}_{nl}$ and (A6) on the left by $\underline{m}_{nl}^{\dagger}$ and subtracting, we get

$$\underline{m}_{nl}^{\dagger}[\underline{G}_{0l}^{(+)}(k_n) - \underline{G}_{0l}^{(+)}(k_n)^{\dagger}]\underline{m}_{nl} = 0 \ . \tag{A8}$$

The symmetry relation

$$\underline{G}_{0l}^{(+)}(k_n) = \underline{G}_{0l}^{(+)}(-k_n^*)^{\dagger}$$

brings (A8) to the form

$$\underline{m}_{nl}(k_n)^{\dagger}[\underline{G}_{0l}^{(+)}(k_n) - \underline{G}_{0l}^{(+)}(-k_n^*)]\underline{m}_{nl}(k_n) = 0 \ . \tag{A9}$$

The matrix in square brackets is anti-Hermitian, and may be brought to diagonal form by means of a unitary transformation. Calling $\tilde{G}_{0l}^{(+)}$ and $\tilde{m}_{nl}$ the transformed quantities,

$$\sum_{s=1}^{N_l} |m_{nls}|^2[\tilde{\underline{G}}_{0l}^{(+)}(k_n) - \tilde{\underline{G}}_{0l}^{(+)}(-k_n^*)]_{ss} = 0 \ .$$

Since $\underline{m}_n \neq 0$, there is at least one value s_0 of the index s for which $|m_{nls}|^2 \neq 0$, then

$$[\tilde{\underline{G}}_{0l}^{(+)}(k_n) - \tilde{\underline{G}}_{0l}^{(+)}(-k_n^*)]_{s_0 s_0} = 0 \ . \tag{A10}$$

Let us write relation (A10) explicitly for the case when $\mathrm{Im}k_n > 0$:

$$2(\mathrm{Re}k_n)(\mathrm{Im}k_n)\int_0^{\infty} \tilde{f}_{s_0}^{(l)*}(q)\frac{1}{[(\mathrm{Re}k_n)^2 - (\mathrm{Im}k_n)^2 - q^2]^2 + 4\mathrm{Re}k_n)^2(\mathrm{Im}k_n)^2}\tilde{f}_{s_0}^{(l)}(q)dq = 0 \ . \tag{A11}$$

Since the integral on the left-hand side of this equation is a positive definite quantity and $\mathrm{Im}k_n > 0$, it follows that

$$\mathrm{Re}k_n = 0 \ . \tag{A12}$$

When $\mathrm{Im}k_n \leq 0$, we get a similar expression in terms of the difference of two positive definite quantities; therefore, for $\mathrm{Im}k_n$ negative or zero, condition (A9) can be satisfied with $\mathrm{Re}k_n \neq 0$.

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