Causality with noncausal optical potentials

V.A. Madsen and K.I. Goldman
Department of Physics, Oregon State University, Corvallis, Oregon 97331
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It is shown by way of a simplified model that the calculation of the time nonlocal potential resulting from an energy-dependent optical potential is not unique. Most choices result in a noncausal time-dependent potential, in spite of the inclusion of appropriate scattering boundary conditions in the model. Similarly, potentials arising from the many-body treatment of the optical potential are typically noncausal. However, it is demonstrated that, because of the energy spectrum of the Hamiltonian, the appropriate wave equations for scattering and the wave-function solutions in both approaches are nevertheless causal.

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I. INTRODUCTION

The subject of time-dependent optical potentials, which was studied in the late 1950s and early 1960s, has recently received new attention in the form of a definitive review article [1] with many physical examples. In Ref. [1], the time-dependent potential $V(t,t')$ is taken to be the Fourier transform of the optical potential, a procedure justified by Coester and Kümmel [2]. The optical potential, from both theoretical and phenomenological viewpoints, is energy-dependent, which makes the potential for the time-dependent Schrödinger equation nonlocal in time. The nonlocality is a simple one, depending only on the time difference $\tau = t - t'$

$$\tilde{V}(t,t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} V(E)\, e^{-iE(t-t')}dE, \qquad (1)$$

where t is the current time and t' is the integration time variable in the potential term of the wave equation,

$$-\frac{\hbar^2}{2m}\nabla^2\psi(t) + \int \tilde{V}(t,t')\psi(t')dt' = i\hbar\frac{\partial\psi(t)}{\partial t}. \qquad (2)$$

One of the more interesting features of the time-dependent Schrödinger equation is its causal nature; i.e., the wave function $\psi(t)$ should not depend on the $\psi(t')$ at later times, $t' > t$. This condition is obviously satisfied if the nonlocal potential itself is causal, that is, if $\tilde{V}(t,t')$ is zero for $t' > t$. Cornwall and Ruderman [3] used the causality of $\psi(t)$ to argue that $\tilde{V}(t,t')$ *must* be causal. We will show in this paper, however, that, although the causality of $\tilde{V}(t,t')$ is a sufficient condition, it is not necessary for the causality of $\psi(t)$. In fact there are whole classes of convenient, exact optical potentials which are noncausal, but still lead to causal behavior of $\psi(t)$.

According to Titchmarsh's theorem, $\tilde{V}(t,t')$ is casual when $\tilde{V}(\tau)$ is the Fourier integral of an energy-dependent potential $V(E)$ which, in the upper half of the complex energy plane, is analytic for finite E and vanishes at $E \to \infty$. In a recent paper [4], we have examined the dispersion, retardation, and causality effects for a simplified special case of the model to be developed in Sec. II. The energy-dependent potential in this model vanishes at $|E| \to \infty$ and is analytic in the finite E plane except for a branch point at the energy of the first excited state of the system and a cut along the real axis from that point to infinity. A curious feature of the calculation of the integral in Eq. (1) is that it involves an integration over very negative energies, where the potential has no physical meaning. Yet, as expected from Titchmarsh's theorem, the resulting integral is causal, and, furthermore, the energy integration to $-\infty$ is absolutely necessary for the proof of causality of $\tilde{V}(\tau)$. In this paper, instead of assuming that the time nonlocal optical potential is the Fourier integral of the energy-dependent potential, we derive it from a simple inelastic-scattering model. We can then show from the result that the unphysical negative energies may be excluded from the energy integral of Eq. (1) but that the resulting time-dependent potentials are noncausal.

The second approach to the optical potential comes from the many-body theory of scattering of nucleons from nuclei. The scattering wave function for elastic scattering of identical particles can be calculated in terms of the one-particle Green's function. The Green's function that follows from the time development of the scattering wave is the particle Green's function. Mahaux and Sartor [5] have found that it is, however, more convenient to work with the time-ordered Green's function, the sum of the particle and hole Green's functions. The addition of the latter (multiplied by any constant) is justified by the authors on the grounds that the hole Green's function does not propagate forward in time and therefore can contribute nothing to the scattering.

The authors argue that in the Fourier transforms they may replace the hole Green's function by a modified one which is the complex conjugate of the hole Green's function below the Fermi energy but precisely equal to the hole Green's function above the Fermi sea. The resulting sum of the particle term and the modified hole term is the retarded Green's function [5,6], which has cuts only in the lower half plane. Thus, according to Titchmarsh's

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theorem, it is causal. In this paper we use the procedure of Ref. [5] to show that the noncausal potentials lead to causal wave functions.

In Sec. II A we first derive an expression for the energy-dependent optical potential, $V(E)$, based on a model consisting of the scattering of a projectile from a target with a number of excited states. In Sec. II B we derive the time-dependent optical potential by writing a time-dependent Schrödinger equation for the projectile plus multiple-channel target system, which is then projected onto the ground-state channel. The result is an expression for the time-dependent potential as an integral of the energy-dependent potential. However, there is considerable freedom of choice of the lower limit E_l on the energy integral because of the finite lower limit on the eigenvalues of the projectile-target system. Referring to the special case of [4], we show that the resulting $\tilde{V}(\tau)$ is noncausal. In Sec. II C we show that, in spite of having a noncausal $\tilde{V}(\tau)$, the potential energy term in the time nonlocal Schrödinger equation is nevertheless causal. Section III discusses the analogous problem in the determination of the optical potential from many-body theory in terms of a one-body Green's function. Section IV contains our conclusions and discussion. Appendix A gives a proof that the energy-dependent model potential of Ref. [4] leads to a noncausal $\tilde{V}(\tau)$ when a finite lower limit on the energy integral is used. Appendix B presents a brief discussion of the analyticity properties of the retarded self-energy operator.

II. SIMPLE MODEL FOR THE OPTICAL POTENTIAL

Here we calculate the energy-dependent optical potential for a particular model of scattering of a nonidentical particle from a target with several excited states, which are formally eliminated to give a one-body Schrödinger equation. We use the potential from this equation to derive the equivalent time-dependent optical potential.

A. Derivation of the energy-dependent optical potential

The wave function for the system of target plus projectile can be expanded in the complete set of eigenstates Φ_n of the target,

$$\Psi(\xi,0) = \sum_{n=0}^{N} \Phi_n(\xi)\, u_n(0), \tag{3}$$

where N is the number of excited states of the target, $n = 0$ referring to the target ground state. Substituting Eq. (3) into the Schrödinger equation, multiplying on the left with $\Phi^\dagger$, and integrating out the internal target coordinate ξ then gives a set of coupled-channels equations,

$$(\mathbf{1}\,E - \mathbf{H})\,\mathbf{u}(E) = 0, \tag{4}$$

where $\mathbf{1}$ is the $(N+1)\times(N+1)$ unit matrix, $\mathbf{H}$ is the Hamiltonian matrix of elements,

$$H_{n,n'} = (h+\epsilon_n)\delta_{nn'} + \langle n|V|n'\rangle, \tag{5}$$

and $\mathbf{u}(E)$ is a column matrix of the coefficient functions $u_n(E)$. In Eq. (5) h is the one-body projectile Hamiltonian.

According to one of the fundamental postulates of quantum mechanics, a general time-dependent state vector may be written as a sum of eigenstates. For our system Eq. (4), the column matrix $\mathbf{u}$ serves as the eigenvector for the system. The time-dependent state vector is then

$$\mathbf{u}(t) = \sum_E A_E\, \mathbf{u}(E)\, e^{-iEt}, \tag{6}$$

where the E sum is used here to designate both a sum over bound states of the projectile-plus-target system and an integration over continuum states of the system. We will retain the summation notation to distinguish the sum over eigenstate energies from other energy integrals which will appear in the following development.

For our purposes it is convenient to turn Eq. (4) into a pair of coupled equations which single out the ground state, onto which we must project our model system to get the theoretical optical potential,

$$(\mathbf{1}E - \mathbf{H}^{(T)})\,\mathbf{u}^{(T)}(E) = \mathbf{V}_{T0}\, u_0(E), \tag{7}$$

$$(E - H_{00})\, u_0(E) = \mathbf{V}_{0T}\, \mathbf{u}^T(E), \tag{8}$$

where the target Hamiltonian, $\mathbf{H}^{(T)}$, is the cofactor matrix of $H_{0,0}$, the ground state matrix element of $\mathbf{H}$, and $\mathbf{V}_{T0}$ is the $N\times 1$ column matrix of target states elements $\langle n|V|0\rangle$ of the projectile-target interaction V.

Equation (7) can then be inverted to give

$$\mathbf{u}^{(T)}(E) = \mathbf{G}^{(T)}\,\mathbf{V}_{T0}\, u_0(E), \tag{9}$$

where $\mathbf{G}^{(T)}(E)$ is an $N\times N$ matrix Green's function,

$$\mathbf{G}^{(T)}(E) = (\mathbf{1}E - \mathbf{H}^{(T)})^{-1}. \tag{10}$$

Generally the Green's function operator will be energy dependent and nonlocal in space, as we see from its definition in Eq. (10). Causality is inserted into the formalism at this point by requiring that the $\mathbf{G}^{(T)}$ of Eq. (10) be an outgoing Green's function, which will ensure that there are only outgoing waves in excited state channels. Substitution of Eq. (9) into Eq. (8) results in

$$(E - H_{00})\, u_0(E) = \mathbf{V}_{0T}\, \mathbf{G}^T(E)\mathbf{V}_{T0}\, u_0(E), \tag{11}$$

the elastic-scattering wave equation we are seeking. It directly involves only the elastic channel, but it contains the energy-dependent dispersive part of the ground-state-channel potential,

$$\Delta M(E) = \mathbf{V}_{0T}\, \mathbf{G}^T(E)\, \mathbf{V}_{T0}, \tag{12}$$

due to the elimination of the excited-state channels. The derivation of Eq. (11) is equivalent, for a nonidentical projectile, to the use of the Feshbach projection of the exact scattering wave equation [7] onto the elastic channel.

B. Derivation of the time-dependent potential

The time-dependent equivalent Schrödinger equation to Eq. (4) for the entire coupled-channels system $\mathbf{u}$ is

$$i\hbar \frac{d\mathbf{u}(r,t)}{dt} = -(\hbar^2/2\mu)\,\nabla^2\,\mathbf{u}(r,t) + \mathbf{V}\,\mathbf{u}(r,t), \quad (13)$$

where $\mathbf{V}$ is the (energy-independent) potential matrix of elements given by the potential term of Eq. (5). To get an equation for the elastic component, we focus on the uppermost (0th) component of Eq. (13). The 0th matrix elements of the two derivative terms contain only u_0, but the potential term couples in all other channel components through the coupling matrix $\mathbf{V}$. Using Eqs. (6) and (9), we may formally eliminate the excited channels and write the 0th component of the potential term of Eq. (13) as follows:

$$i[\mathbf{V}\,\mathbf{u}(r,t)]_0 = \sum_E A_E \left[V_{0,0} + \sum_{n,n'} V_{0,n}\, G^{(T)}_{n,n'}(E)\, V_{n',0} \right] \times u_0(r,E)\, e^{-iEt/\hbar}. \quad (14)$$

Not surprisingly, we recognize in the second term of the right-hand side of Eq. (14) the dynamic potential, $\Delta M(E)$, of Eq. (12). For the first term of Eq. (14) we may factor $V_{0,0}$ out of the sum to get $V_{0,0}\,u_0(r,t)$. The Green's function makes the second term generally nonlocal in space. Because of its energy-dependence, we may not factor the Green's function and potential factors out of the E sum, which leads us also to a nonlocality in time, as we now demonstrate with the help of the Dirac δ function relationship,

$$\int_{-\infty}^{\infty} e^{i(E'-E)t'}\,dt' = 2\pi\delta(E'-E). \quad (15)$$

Thus we may write the dynamic potential term of Eq. (14) as

$$\begin{aligned}
&\sum_E A_E \int_{E_l}^{\infty} \Delta M(E')\,u_0(r,E) e^{-iE't} \left[(2\pi)^{-1} \int_{-\infty}^{\infty} e^{i(E'-E)t'}\,dt' \right] dE' \\
&\quad = \sum_E \int_{-\infty}^{\infty} (2\pi)^{-1} \int_{E_l}^{\infty} e^{-iE'(t-t')} \Delta M(E')\,dE'\; A_E\,u_0(r,E)\,e^{-iEt'}\,dt' \\
&\quad = \int_{-\infty}^{\infty} \Delta\tilde{M}(t,t')\,u_0(r,t')\,dt', \quad (16)
\end{aligned}$$

where

$$\Delta\tilde{M}(t,t') = (2\pi)^{-1} \int_{E_l}^{\infty} e^{-iE'(t-t')}\,\Delta M(E')\,dE', \quad (17)$$

is the time nonlocal potential arising from the energy-dependence of Eq. (12) and E_l is any lower limit on the eigenvalues of the combined system of target and projectile. Contributions to the E' integral from below the lowest eigenvalue do not add anything to Eq. (16) since the t' integral gives back the $\delta(E-E')$, which will be zero in any domain of E' not including an eigenenergy included in the E sum of Eq. (6). Note that $\Delta\tilde{M}(t,t')$ depends only on the difference τ between the current time t and the nonlocal integration variable t' of Eq. (16).

A possible choice of E_l is $-\infty$, which makes $\Delta\tilde{M}(t,t')$ the Fourier transform of $\Delta M(E)$. In [4] it was shown explicitly that a special case of the model presented in Sec. II A led to a causal potential for $E_l = -\infty$. Indeed, the energy-dependent potential for that case satisfies Titchmarsh's theorem, which then implies that the Fourier transform is causal. In Appendix A it is shown explicitly that the energy-dependent potential from [4] with a finite lower limit leads to a noncausal potential.

We may think of Eq. (17) as giving the Fourier integral of a function $\Delta M(E')$ which for complex E' has a zero value for $\mathrm{Re}\,E' < E_l$, leading to exactly the same integral. Such a function would, of course, not be analytic in the upper half plane (analytic functions have only isolated zeros) and would therefore fail to satisfy the conditions of Titchmarsh's theorem.

Using Eq. (17) we may write the zeroth (elastic) component of Eq. (13) as

$$i\hbar \frac{\partial u_0(r,t)}{\partial t} = -(\hbar^2/2\mu)\,\nabla^2\,u_0(r,t) + V_{0,0}u_0(r,t) + \int_{-\infty}^{\infty} \Delta\tilde{M}(t,t')\,u_0(r,t')\,dt'. \quad (18)$$

This is the time-dependent Schrödinger equation for the elastic channel, corresponding to Eq. (2). The first potential term is a static potential, and the second one is a time-dependent, time nonlocal potential.

C. Causality of the time-dependent Schrödinger equation

According to Eq. (17), the time-dependent nonlocal optical potential $\Delta\tilde{M}(t,t')$ need not be the Fourier in-

tegral of the energy-dependent optical potential. If the lower limit on the integration is chosen to be $-\infty$, the energy integral of Eq. (17) is the Fourier transform, and then the $M(t,t')$ is zero for $t' > t$; i.e., it is causal. Otherwise, for a finite lower limit, it is generally noncausal.

The dispersive part of the optical potential term in the time-dependent Schrödinger equation for elastic scattering, according to Eqs. (17) and (18), is

$$\begin{aligned}\int_{-\infty}^{\infty} \Delta\tilde{M}(t,t')\,\psi(t')\,dt' &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{E_l}^{\infty} e^{-iE'(t-t')}\Delta M(E')\,dE'\,\psi(t')\,dt' \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-iE'(t-t')}\Delta M(E')\,dE'\psi(t')\,dt' - \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{E_l} e^{-iE'(t-t')}\Delta M(E')\,dE' \\ &\quad \times \sum_E A_E\,\psi(E)\,e^{-iEt'}\,dt', \end{aligned} \tag{19}$$

where in the last term the eigenfunction expansion of $\psi(t')$, replacing u_0 of Eq. (6), has been used for the elastic channel. Integrating over t' gives us for the last term of Eq. (19),

$$\frac{1}{2\pi}\int_{-\infty}^{E_l} e^{-iE't}\,\Delta M(E')\,dE' \sum_E A_E\,\psi(E)\,\delta(E-E'), \tag{20}$$

which is zero, since the lowest eigenvalue $E \equiv E_0 > E_l$, by definition of E_l. Thus,

$$\begin{aligned}&\int_{-\infty}^{\infty} \Delta\tilde{M}(t,t')\,\psi(t')\,dt' \\ &\quad = \int_{-\infty}^{\infty} \frac{1}{2\pi}\left[\int_{-\infty}^{\infty} e^{-iE'(t-t')}\Delta M(E')\,dE'\right]\psi(t')\,dt'. \end{aligned} \tag{21}$$

The quantity in the brackets of Eq. (21) is essentially the Fourier integral version of the time-dependent optical potential, which, according to Titchmarsh's theorem, is causal. The causal potential forces causality on the wave function $\psi(t)$ since it cuts off the integration over $t' > t$. Thus we have showed that, even though the original form of the time-dependent optical potential is not itself causal, the potential term in the time-dependent wave equation and, therefore, the wave function are still causal.

III. NONCAUSAL POTENTIALS FROM MANY-BODY THEORY

In the many-fermion approach to the nuclear optical model [5,8,9], the wave function can be related to the one-body Green's function and the optical potential to the self-energy operator. Mahaux and Sartor [5,10] have pointed out that this optical potential may be noncausal. In this section we give a packet version of this development and show that the noncausal potential leads to a causal equation of motion and wave function.

A. Packet development of the scattering problem

We make up a packet F for the projectile at a starting time t_0, such that $F(r,t_0)$ and the target nucleus are completely separated at $t = t_0$. Thus, although the interaction is on, it is ineffective in scattering until much later when the packet encounters the target. We also assume that the packet is sharply peaked around some definite momentum, so it has to be long in the spatial dimension. This requires two scales of length, l_p for the packet length and L_0 for the packet-target distance, which must satisfy the condition $L_0 \gg l_p$. The state vector of the projectile-target system at time t_0 is then

$$|\Psi^{A+1}(t_0)\rangle = e^{-iE_0t_0}\int d^3r\,F(r,t_0)\,\psi^\dagger(r)\,|\Psi_0\rangle, \tag{22}$$

where here $\psi^\dagger(r)$ is the creation operator for a particle at point r and $|\Psi_0\rangle$ and E_0 are the (time-independent) ground-state (GS) eigenfunction and energy eigenvalue of the A-particle system. The phase factor $e^{-iE_0t_0}$ is included for later convenience in writing the elastic scattering wave function in terms of the one-particle Green's function.

Next we substitute a Fourier integral,

$$F(r,t_0) = \int d^3k\,\tilde{F}(k,t_0)\,e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{23}$$

into Eq. (22) and integrate over r to obtain for the initial state vector

$$|\Psi^{A+1}(t_0)\rangle = e^{-iE_0t_0}\int d^3k\,\tilde{F}(k,t_0)\,a^\dagger(k)\,|\Psi_0\rangle, \tag{24}$$

where $a^\dagger(k)$ creates a particle in a plane-wave state k.

The initial state vector of the scattering wave function in terms of the Fourier integral, Eq. (24), is an expansion in the complete set of plane wave eigenstates of the free-particle Hamiltonian. It is shown in Merzbacher's text [11] that the initial packet in scattering from a static potential U can equally well be written in terms of an expansion in scattering eigenstates $\psi_k^{(+)}$ of the Hamiltonian H_0 consisting of the kinetic energy operator plus U, where k is the wave vector of the input plane wave part of ψ. Furthermore, the Fourier coefficient in terms of the scattering wave expansion is precisely equal to the $\tilde{F}(k,t_0)$ of the plane-wave expansion in Eq. (24).

In principle, an expansion in terms of eigenstates of a scattering Hamiltonian, must include both the continuum (scattering) states κ and the bound states α.

However, the coefficients for the bound states are essentially zero, because the large initial separation L_0 between the projectile and the target makes the overlap between the initial packet and the bound states of the scattering Hamiltonian virtually zero. The use of the static auxiliary potential U is important for the later development in terms of the Green's function to hold the nucleons together in the unperturbed ground state. Following the notation of Mahaux and Sartor [5], we label the eigenstates of the auxiliary potential with quantum number index α. However, when α designates a state in the continuum, we use the wave number of the plane-wave part of the scattering eigenstate as the quantum number but call it κ to distinguish it from the momentum index k used to designate a plane wave state. Thus the initial state vector, Eq. (24), in terms of the scattering eigenstates is rewritten as

$$|\Psi^{A+1}(t_0)\rangle = e^{-iE_0t_0}\int d^3\kappa\,\tilde{F}(\kappa,t_0)\,a^\dagger(\kappa)\,|\Psi_0\rangle. \quad (25)$$

The wave function at later times is then given with the use of the time development operator by

$$\Psi^{A+1}(t) = e^{-iE_0t_0}e^{-iH(t-t_0)}\int d^3\kappa\tilde{F}(\kappa,t_0)\,a^\dagger(\kappa)\,|\Psi_0\rangle. \quad (26)$$

To make an energy analysis of Eq. (26) we may expand in eigenstates n of the $(A+1)$-particle system

$$|\Psi(t)\rangle = e^{-iE_0t_0}\sum_n e^{-iE_n(t-t_0)} \times\int d^3\kappa\,\tilde{F}(\kappa,t)\,|\Psi_n^{A+1}\rangle\langle\Psi_n^{A+1}|\,a^\dagger(\kappa)|\Psi_0\rangle, \quad (27)$$

where, as in Eq. (6), the sum includes continuum components of the $(A+1)$-nucleon system. Because the packet was prepared by adding a continuum particle to the ground state of the target beyond the range of the interaction, all energy components n of the initial state have *positive energies with respect to the ground state of the target.* This energy distribution is preserved by the energy conserving total Hamiltonian H as the packet develops, as shown in Eq. (27).

From the initial time t_0, Eq. (26) gives the exact development of the state vector as the projectile approaches, interacts with, and recedes in all directions from the target. It will include, for large t, all excited states of the target and all reaction products within the energy domain of the projectile packet. For describing elastic scattering we must project from that complicated scattered wave its elastic component. We wait patiently until all reaction products (which may include photons from nucleons which have been radiatively captured by the target) have escaped the target region and the remainder of the incident wave has passed on. At this time the projectile packet is no longer interacting with the target, so we may project out the elastic component by taking the overlap of the exact scattered wave with potential scattering states incident on the nucleus in its ground state, $a^\dagger(\kappa')\,|\Psi_0\rangle e^{-iE_0t}$. This process leaves a one-particle wave function in the space of the eigenstates of the (auxiliary) potential. Equation (26) gives

$$\begin{aligned} e^{iE_0t}\langle\Psi_0|\,a(\kappa')\,|\Psi^{A+1}(t)\rangle &= e^{iE_0(t-t_0)}\int d^3\kappa\,\tilde{F}(\kappa,t_0)\,\langle\Psi_0|a(\kappa')\,e^{-iH(t-t_0)}\,a^\dagger(\kappa)\,|\Psi_0\rangle, \\ &= \int d^3\kappa\tilde{F}(k,t_0)\,\langle\Psi_0\,|\,e^{iHt}a(\kappa')\,e^{-iH(t-t_0)}\,a^\dagger(\kappa)\,e^{-iHt_0}|\Psi_0\rangle, \\ &= \int d^3\kappa\,\tilde{F}(\kappa,t_0)\langle\Psi_0\,|\,a(\kappa',t)\,a^\dagger(\kappa,t_0)\,|\,\Psi_0\rangle, \end{aligned} \quad (28)$$

where $a(\kappa',t)$ is the destruction operator in the Heisenberg picture. By comparison the one-body time-ordered Green's function [5,9] is

$$G(\kappa',\kappa,t-t_0) = -i\theta(t-t_0)\,\langle\Psi_0\,|\,a(\kappa',t)\,a^\dagger(\kappa,t_0)\,|\,\Psi_0\rangle + i\theta(t_0-t)\,\langle\Psi_0\,|a^\dagger(\kappa,t_0)\,a(\kappa',t)\,|\,\Psi_0\rangle. \quad (29)$$

The first and second terms on the right will be referred to later as the particle and hole Green's functions, respectively. From the derivation of Eq. (28) it is clear that $t > t_0$, so the step function factor in Eq. (29) multiplies the matrix element in the first term of Eq. (29) by 1 and the matrix element in the second term by 0. Thus for times relevant for the scattering of the packet, Eq. (26),

$$\langle\Psi_0\,|\,a(\kappa',t)\,a^\dagger(\kappa,t_0)\,|\,\Psi_0\rangle = iG(\kappa',\kappa,t-t_0). \quad (30)$$

B. Dyson's equation and the Lippmann-Schwinger equation

Dyson's equation [5,9], for the Green's function, Eq. (29), is

$$\begin{aligned} G(\kappa',\kappa,t-t_0) = G^0(\kappa',\kappa,t-t_0) + \int\int G^0(\kappa',\kappa'',t-t')\int\int[N(\kappa'',\kappa''',t'-t'') - U(\kappa'',\kappa''')\delta(t'-t'')] \\ \times G(\kappa''',\kappa,t''-t_0)\,d^3\kappa'''dt''d^3\kappa''dt', \end{aligned} \quad (31)$$

where N is the particle self-energy or mass operator. The static auxiliary potential U appears subtracted from the self-energy to compensate for its inclusion in H_0. The delta function $\delta(t'-t'')$ is the time dependence of U expressed as a nonlocal operator.

The unperturbed Green's function appearing in the first term on the right-hand side of Eq. (31) is

$$G^0(\kappa',\kappa,t-t_0) = -i\theta(t-t_0)\langle\Phi_0|a_0(\kappa',t)\,a_0^\dagger(\kappa,t_0)|\Phi_0\rangle + i\theta(t_0-t)\langle\Phi_0|a_0^\dagger(\kappa,t_0)a_0(\kappa',t)|\Phi_0\rangle, \tag{32}$$

where $a_0^\dagger$ is a creation operator in the interaction picture,

$$a_0^\dagger(\kappa,t_0) = e^{iH_0t_0}a^\dagger(\kappa)e^{-iH_0t_0} = e^{i\epsilon_\kappa t_0}a^\dagger(\kappa), \tag{33}$$

and $|\Phi_0\rangle$ is the unperturbed ground state of the A-particle system. In this case $|\Phi_0\rangle$ is the independent-particle ground state in the auxiliary binding potential $U(\kappa',\kappa)$.

The second term in Eq. (32) is zero because $a_0(\kappa',t)$ is the destruction operator for a continuum particle while $|\Phi_0\rangle$ has only bound single-particle states. It can be replaced by another zero term to give the unperturbed Green's function, Eq. (32), in the form

$$\begin{aligned} G^0(\kappa',\kappa,t-t_0) &= -ie^{-i(\epsilon_{\kappa'}t-\epsilon_\kappa t_0)}\theta(t-t_0)\langle\Phi_0|a_0(\kappa')a_0^\dagger(\kappa) + a_0^\dagger(\kappa)a_0(\kappa')|\Phi_0\rangle \\ &= -i\,\theta(t-t_0)\delta^3(\kappa-\kappa')\,e^{-i\epsilon_\kappa(t-t_0)}. \end{aligned} \tag{34}$$

The right-hand side of Eq. (34) for $t > t_0$ is exactly the form of the time-dependent unperturbed wave function for scattering in the auxiliary potential multiplied by the phase factor $-ie^{i\epsilon_\kappa t_0}$.

Now, if Dyson's equation for scattering is solved by iteration, the factor $G(\kappa''',\kappa,t''-t_0)$ in Eq. (31) will get replaced by the entire right-hand side of the equation, evaluated at appropriate time and wave vector arguments, which has Eq. (34) as its first term. In each term of the iteration there will appear a phase factor $e^{-i\epsilon_\kappa(t_n-t_0)}$, where t_n is some integrated time. The constant phase factor $-ie^{i\epsilon_\kappa t_0}$ will be common to every term and may be divided out.

We next determine the Fourier transform of the time-dependence of the resulting equation, first taking the limit that $t_0 \to -\infty$. To start, in this limit the Fourier transform of the G^0 term, Eq. (34), is

$$\begin{aligned} G^0(\kappa',\kappa,\omega) &= -i(2\pi)^{-1}\lim_{t_0\to-\infty}\int G^0(\kappa',\kappa,t)e^{i\omega t}dt \\ &= -ie^{i\epsilon_\kappa t_0}\delta^3(\kappa-\kappa')\,\delta(\omega-\epsilon_\kappa). \end{aligned} \tag{35}$$

Since every term of the time-dependent equation will have a factor $e^{-i\epsilon_\kappa t_n}$, every term of the right-hand side of the Fourier transformed equation will have a common factor $\delta(\omega-\epsilon_\kappa)$. The Fourier transform of the Dyson equation, divided by $-ie^{i\epsilon_\kappa t_0}$, taken in the limit of $t_0 \to -\infty$, and integrated over a small domain of ω containing ϵ_κ, is then

$$\begin{aligned} \psi(\kappa',\kappa,\epsilon_\kappa) = \delta^3(\kappa'-\kappa) &+ \int G^0(\kappa',\kappa'',\epsilon_\kappa) \\ &\times\int[N(\kappa'',\kappa''',\epsilon_\kappa) - U(\kappa'',\kappa''')] \\ &\times\psi(\kappa''',\kappa,\epsilon_\kappa)\,d^3\kappa'''d^3\kappa'', \end{aligned} \tag{36}$$

with the δ-function term coming from Eq. (35) and ψ defined in terms of the Fourier transform of G,

$$\psi(\kappa',\kappa,\omega)\delta(\omega-\epsilon_\kappa) = \lim_{t_0\to-\infty}(-ie^{i\epsilon_\kappa t_0})^{-1}G(\kappa',\kappa,\omega). \tag{37}$$

Note that Eq. (31) is not an equation for the entire Green's function, which also has bound matrix elements. However the scattering problem requires only the continuum components of G_p, which are covered completely by the left-hand side of Eq. (36). Bound internal quantum numbers will occur as part of the κ''' integral in the right-hand side of Eqs. (31) and (36); i.e., κ''' runs over all single-particle states, which may include some bound states, in which case the κ''' integrals must be interpreted as including discrete sums.

For the integral term of Eq. (36) we need also to evaluate the zero-order Green's function G^0, the first factor in the integral term on the right. However, in the interest of relating the Dyson equation to scattering theory we first write the zero-order Green's function for scattering in momentum space,

$$g(k',k,\omega) = \sum_\alpha \frac{\chi_\alpha^+(k')\,\chi_\alpha^{+*}(k)}{\omega-\epsilon_\alpha+i\eta} + \int d^3\kappa\frac{\chi_\kappa^+(k')\,\chi_\kappa^{+*}(k)}{\omega-\epsilon_\kappa+i\eta}, \tag{38}$$

where the sum is over bound states of the auxiliary potential and the integral is over the continuum of its scattering states. The κ',κ'' element of the Eq. (38), with κ' in the continuum, is

$$g(\kappa',\kappa'',\omega) = \frac{\delta^3(\kappa'-\kappa'')}{\omega-\epsilon_{\kappa'}+i\eta}. \tag{39}$$

By comparison the zero-order one-body Green's function is

$$\begin{aligned} G^0(\kappa',\kappa'',t-t') &= -ie^{-i(\epsilon_{\kappa'}t-\epsilon_{\kappa''}t')}[\theta(t-t')\langle\Phi_0\,|\,a_0(\kappa')\,a_0^\dagger(\kappa'',)\,|\,\Phi_0\rangle - \theta(t'-t)\langle\Phi_0\,|\,a_0^\dagger(\kappa'',)\,a_0(\kappa')|\Phi_0\rangle] \\ &= -i\,\theta(t-t')\delta^3(\kappa'-\kappa'')e^{-i\epsilon_{\kappa'}(t-t')}. \end{aligned} \tag{40}$$

The second term in this Green's function, which is again zero because the continuum destruction operator operates only on bound single-particle states in $|\Phi_0\rangle$, has been altered in the evaluation by changing the coefficient from $-\theta(t'-t)$ to $+\theta(t-t')$. Thus the Fourier transform of Eq. (40) is equal to the zero-order scattering Green's function, Eq. (39),

$$G^0(\kappa',\kappa'',\omega) = g(\kappa',\kappa'',\omega), \tag{41}$$

which allows us to replace the G^0 in Eq. (36) by the scattering Green's function $g(\kappa',\kappa'',\omega)$. With this change Eq. (36) has exactly the form of the Lippmann-Schwinger integral equation for scattering. The delta function $\delta^3(\kappa-\kappa')$ is precisely the expression for a potential scattering eigenfunction κ at scattering-eigenstate coordinate κ', giving component κ of the incident packet in Eq. (25). Equation (36) is the Lippmann-Schwinger equation for scattering by two potentials in the auxiliary-potential eigenstate basis. The first term is the wave function for scattering from the auxiliary potential $U(\kappa',\kappa)$, and the integral gives the effects on the wave function of the scattering from the second potential, $N(\kappa',\kappa,\epsilon_\kappa)-U(\kappa',\kappa)$. The derivation of the Lippmann-Schwinger equation in this many-body approach [5,8,9] established the relationship Eq. (37) as the connection between the Green's function and the wave function for elastic scattering. It also established $N(\kappa'',\kappa''',\epsilon_\kappa)$ as the potential responsible for elastic scattering, that is, the optical potential.

However, as mentioned in the Introduction to this section, Mahaux and Sartor have pointed out that the self-energy N is not causal, which might give rise to some concern about using it to describe scattering via Eq. (36). A similar phenomenon was encountered in Eq. (17). Analogous to the development in Sec. II, we will show that the use of the noncausal N still gives rise to a causal Lippmann-Schwinger equation for scattering. For this purpose it is useful first to discuss the analytic properties of the Green's function.

C. Analytic properties of the Green's functions

To proceed further with the argument about causality we consider the spectral representation [12] of the particle and hole Green's functions,

$$G_{p,\beta,\alpha}(\omega) = \sum_{n,\nu} \frac{\langle\Psi_0 \mid a_\beta \mid \Psi_n^{A+1,\nu}\rangle\langle\Psi_n^{A+1,\nu} \mid a_\alpha^\dagger \mid \Psi_0\rangle}{\omega - E_n^{A+1,\nu} + E_0^A + i\eta}, \tag{42}$$

$$G_{h,\beta,\alpha}(\omega) = \sum_{n,\nu} \frac{\langle\Psi_0 \mid a_\alpha^\dagger \mid \Psi_n^{A-1,\nu}\rangle\langle\Psi_n^{A-1,\nu} \mid a_\beta \mid \Psi_0\rangle}{\omega + E_n^{A-1,\nu} - E_0^A - i\eta}, \tag{43}$$

where α and β designate the single-particle quantum numbers and ν designates the nucleon type (neutron or proton) added to or removed from the ground state of the A-particle system. The two denominators can be written as [12]

$$\omega - E_n^{A+1,\nu} + E_0^{A+1,\nu} - E_0^{A+1,\nu} + E_0^A + i\eta = \omega - \epsilon_n^{A+1,\nu} + S^{A+1,\nu} + i\eta, \tag{44}$$

$$\omega + E_n^{A-1,\nu} - E_0^{A-1,\nu} + E_0^{A-1,\nu} - E_0^A - i\eta = \omega + \epsilon_n^{A-1,\nu} + S^{A,\nu} - i\eta, \tag{45}$$

where $S^{A,\nu}$ is the separation energy of a nucleon of type ν from an A-nucleon system and $\epsilon_N^{A\pm1}$ is the excitation energy in the $A\pm1$ nucleon system. The analytic behavior of the particle and hole Green's functions in the complex energy plane is represented [12] by Fig. 1. The particle Green's function has a series of poles starting at $\omega = -S^{A+1,\nu} - i\eta$, extending to the right to the pole of the highest ν-nucleus bound state, then, as the particle continuum is reached, turning into a cut, which extends from $\omega = -i\eta$ to $+\infty - i\eta$. The hole Green's function has a series of poles starting at $\omega = -S^{A,\nu} + i\eta$, extending left to the continuum of the $A-1$ system at $\omega = -S^{A-1,\nu} - S^{A,\nu} + i\eta$ and continuing as a cut to $-\infty + i\eta$.

In the limit of an infinite nucleus in the absence of pairing, $S^{A+1,\nu}$ and $S^{A,\nu}$ will be equal, but in finite nuclei they will not. They may differ by a few MeV due to pairing and shell effects. However, the zero in the scattering energy starts at the continuum cut of G_p, where $\epsilon_n^{A+1,\nu} = S^{A+1,\nu}$. According to Eq. (44) and the previous paragraph, the start of this cut is at $\mathrm{Re}\,\omega = 0$, so $\mathrm{Re}\,\omega + \epsilon_N^{A-1,\nu} + S^{A,\nu}$ in the denominator Eq. (45) of Eq. (43) will be positive definite, since $\epsilon_n^{A-1,\nu} > 0$ and $S^{A,\nu}$ is positive and finite, making the $-i\eta$ term negligible in the limit as η approaches zero. Thus with absolutely no change at positive energies we may replace the minus sign in front of the $i\eta$ to a plus sign, which changes $G_h(\omega)$ to $G_h^\dagger(\omega^*)$. Although G_h and $G_h^\dagger(\omega^*)$ will be unequal for $\mathrm{Re}\,\omega < 0$, they will be equal in the scattering region. In $G_h^\dagger(\omega^*)$, the hole cut will switch from above to below the real ω axis. It is convenient at this point to introduce the retarded Green's function [5,6]

$$G^R(\omega) = G_p(\omega) + G_h^\dagger(\omega^*) \tag{46}$$

which will have cuts only in the lower half plane, as shown in Fig. 2. The analytic properties of the self-energy N^R

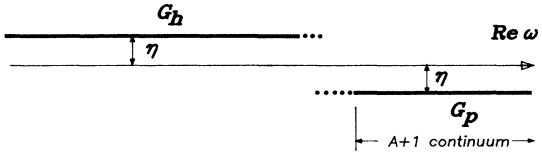

FIG. 1. The pole and cut structure of the time-ordered Green's function in the complex energy plane.

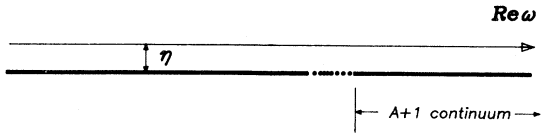

FIG. 2. Same as Fig. 1 for the retarded Green's function.

for the Green's function G^R are discussed in Appendix B. Like G^R, it is analytic in the upper half plane and has cuts in the lower half plane, which coincide with those of G^R.

D. Causal behavior from noncausal potentials

Even though N is noncausal, Eq. (36) does, nevertheless, lead to causal behavior. Since in the scattering energy region $\omega > 0$, $G(\omega)$ and $G^R(\omega)$ are equal, as shown in Sec. III C, so are $N(\omega)$ and $N^R(\omega)$, which follows from Eqs. (B2) and (B3) and the discussion following them in Appendix B. Therefore we may substitute N^R for N in Eq. (36) and G^R for G in Eq. (37) without changing either equation at scattering energies. This procedure gives a nearly identical Lippmann-Schwinger equation,

$$\psi(\kappa',\kappa,\epsilon_\kappa) = \delta^3(\kappa-\kappa') + \int\int g(\kappa',\kappa'',\epsilon_\kappa) \times[N^R(\kappa'',\kappa''',\epsilon_\kappa) - U(\kappa'',\kappa''')]\psi(\kappa''',\kappa,\epsilon_\kappa)d^3\kappa'''d^3\kappa'', \quad (47)$$

where advantage was taken of the equivalence of the zero-order Green's functions, Eq. (41). However, in Eq. (47) the retarded self-energy N^R appears in the role as the scattering potential instead of N. Its Fourier integral,

$$N^R(\kappa',\kappa,\tau) = \int N^R(\kappa',\kappa,\omega)\, e^{-i\omega\tau} d\omega \quad (48)$$

will be causal,

$$N^R(\kappa'',\kappa''',t'-t'') = 0, \quad t'' > t'. \quad (49)$$

The time-dependent equivalent to Eq. (47),

$$\psi(\kappa',\kappa,t) = \delta^3(\kappa-\kappa')e^{-i\epsilon_\kappa t} + \int\int g(\kappa',\kappa'',t-t')\int\int[N^R(\kappa'',\kappa''',t'-t'') - U(\kappa'',\kappa''')\delta(t'-t'')] \times\psi(\kappa''',\kappa,t'')d^3\kappa'''\,dt''\,d^3\kappa''\,dt', \quad (50)$$

has three causal functions $N^R(\kappa'',\kappa''',t'-t'')$, $\delta(t'-t'')$, and

$$g(\kappa',\kappa'',t-t') = 0, \quad t' > t \quad (51)$$

in the time integration. Thus the integral over t'' is effectively limited by Eq. (49) and the delta function to the range $t'' \le t'$ and t' is limited by Eq. (51) to the range $t' \le t$. The integrand is therefore nonzero only for $t'' \le t$; that is, the time-dependent Lippmann-Schwinger equation, Eq. (50), is causal.

We emphasize that we have not replaced Eq. (36) by a different equation Eq. (47), which is causal. We have started with Eq. (36), including its noncausal potential N and substituted the equal quantities G^R and N^R for G and N, leaving exactly the same equation (at scattering energies) as we started with but with N^R appearing instead of N. Since N^R is causal, so is ψ. Thus a Lippmann-Schwinger equation with a noncausal potential leads to a causal scattering wave function. This result corresponds very closely to the proof of causality for the noncausal potential of Eq. (17). In both cases we start with a noncausal time-dependent potential and equate it to a causal one, the change not affecting the wave equation at scattering energies.

E. A continuum of noncausal potentials

Mahaux and Sartor [5] define a one-particle Green's function which has a variable amount of hole Green's function:

$$G(k',k,t-t',a) = G_p(k',k,t-t') + a\,G_h(k',k,t-t'), \quad (52)$$

$$G^0(k',k,t-t',b) = G^0_p(k',k,t-t') + b\,G_h(k',k,t-t'), \quad (53)$$

where again the particle and hole Green's functions are, respectively, the forward and backward propagating parts of the time-ordered Green's function, Eq. (29). Mahaux and Sartor postulate that these Green's functions Eqs. (52) and (53) can be made to satisfy a generalized Dyson-like equation, a special case of which is

$$G(\kappa',\kappa,\omega,a) = G^0(\kappa',\kappa,\omega,b) + \int\int G^0(\kappa',\kappa'',\omega,1) \times[N(\kappa'',\kappa''',\omega,a,b) - U(\kappa'',\kappa''')] \times G(\kappa''',\kappa,\omega,a)d^3\kappa''d^3\kappa''', \quad (54)$$

where the last two arguments of N specify which of the choices from Eqs. (52) and (53) were made. Writing Eq. (31) as a matrix expression, the authors solve for the self-energy $N(a,b)$, the only assumption being that the inverses of Eqs. (52) and (53) exist. The result with $b = 1$ is

$$N_{\mu,\nu}(a,1) - U = (\omega - e_\mu)\delta_{\mu\nu} - G^{-1}_{\mu\nu}(a). \quad (55)$$

The optical potential, established in Eq. (36) as the self-energy operator, is expected to have the same analytic properties [5] as the Green's function itself. The Fourier transform of the particle Green's function has only a right-hand cut, which lies below the real axis of the ω plane while the hole Green's function has a left hand cut, which lies above the real axis. Thus, according to Titchmarsh's theorem, the particle Green's function is causal. On the other hand, any choice of Green's function with $a \neq 0$ in Eq. (52), for example the time-ordered Green's function, $a = 1$, has also the left-hand cut. Any choice of $a \neq 0$ will therefore give a noncausal potential, as it violates Titchmarsh's theorem. Since the multiplying constant a is arbitrary, there is a continuum of noncausal potentials. However one may again use the arguments of the previous section, changing the sign of the η term in G_h of Eq. (43) from negative to positive. Again this changes nothing at positive energies ω, but converts $G(a)$ to $G^R(a)$, which is analytic in the upper half plane. The proofs given in Refs. [13] and [14] that G has no zeros in the upper half ω plane can be extended to Eq. (52), provided only that $a \geq 0$, to maintain the negative definiteness of its imaginary part, and likewise for G^0. Thus, the retarded analog of Eq. (55) holds, and the retarded self-energy can be calculated. As it is analytic in the upper half plane, the time-dependent N^R will be causal for all positive values of the parameters a and b.

This phenomenon is similar to the result described above in Sec. II B, summarized in Eq. (17). The continuum of values of E_l all lead to the same scattering, but only the choice $E_l = -\infty$ of these leads to a causal potential. In Sec. II C we showed that these time-dependent optical potentials lead, nevertheless, to causal behavior of the wave function.

IV. SUMMARY AND CONCLUSIONS

We have determined the time nonlocal optical potential for two models of elastic scattering. The first is a simple reaction model of scattering with a nonidentical projectile from a target with any number of excited states. The time-dependent potential, given by a Fourier integral of the energy-dependent optical potential resulting from the model, is the one which appears in the time-dependent Schrödinger equation. Because of the finite lower limit on the spectrum of the complete system of projectile and particle, the lower limit of the integral is indefinite. In principle, it can be chosen to have any value of energy below the lowest energy eigenvalue. As a practical matter, it can have any energy value below zero scattering energy, since only positive energies appear in the incident packet wave function.

In Refs. [1,4] the lower limit was taken to be $-\infty$, which makes the time-dependent potential equal to the Fourier integral of the energy-dependent optical potential. Titchmarsh's theorem then applies, resulting in a causal potential. The proof of causality for a special case of our model potential, for which the proof was carried out explicitly [4], also required the infinite lower limit.

We have shown in Appendix A of this paper that, if a finite lower limit is taken, the time-dependent potential is not generally causal. This was done by actually carrying out numerically the integral of Eq. (17) for the special simplified case of Ref. [4]. It is, of course, no surprise that this potential is noncausal, as it violates Titchmarsh's theorem.

However, we have shown that, in spite of the noncausal nature of the potentials, the time-dependent Schrödinger equation (and therefore the wave function) is still causal. In the scattering theory, before projection on the elastic channel, causality was inserted in the form of outgoing scattered waves in the excited channels of the target nucleus. Although the derivation of the wave equation in the elastic channel does give rise to noncausal potentials in the sense that $V(t,t') \neq 0$ $t' > t$, these potentials still lead to causal behavior.

In addition, we have presented a many-body treatment of the optical potential using a packet description of the scattering. We have shown that the noncausal potential which arises [5] from the derivation of the Lippmann-Schwinger equation from the Dyson equation also results in a causal wave equation. This has been accomplished by converting the equation of motion to one involving the retarded Green's function and self-energy. Both of these quantities satisfy Titchmarsh's theorem, thereby giving rise to a causal time-dependent Lippmann-Schwinger equation describing the scattering. We have included in Appendix B a brief discussion of the analyticity properties of the retarded Green's function and self-energy.

Both cases we have discussed result in an equation of motion containing a noncausal time nonlocal optical potential. In each case the potential may be altered by making adjustments in the the corresponding energy-dependent potential (its Fourier transform). The alteration is justified because it makes a difference only at negative energies with respect to the ground state of the target, whereas only positive energies are contained in the scattering wave packet.

One could take the point of view that the noncausal potentials we have discussed are actually causal, as they lead to causal behavior in the wave function. All the optical potentials we have discussed satisfy this criterion. We have used the more restrictive definition of a causal potential, that $V(t,t') = 0$ for $t' > t$. The fact that our noncausal potentials have led to causal behavior depends on the fact that they are each identical to causal potentials at scattering energies. Our proof that they lead to causal behavior in each model relies on the existence of causal potentials into which the noncausal potentials may be converted by manipulation of the potential and wave function in the negative energy domain. As the scattering packet contains none of the negative scattering energies, the change in the energy-dependence of the potential below zero energies does not affect the scattering wave function. Since in each case the substituted potential satisfies Titchmarsh's theorem, the corresponding time-dependent potential is causal. The substituted potential then gives rise to a causal wave equation, the solution of which is a causal wave function.

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APPENDIX A: NONCAUSALITY OF THE OPTICAL POTENTIAL FROM A SIMPLE REACTION MODEL

In this appendix, the noncausal nature of a special case of Eq. (17) will be demonstrated. The optical potential, which is forced to be spatially local by restricting the scattering model to inelastic scattering on a spherical shell of potential, is [4]

$$\Delta M(E) = \frac{e^{ikr}\sin(kr)\,\delta(r-a)}{k}, \tag{A1}$$

where $k = \sqrt{E}$. We demonstrate here that $\Delta\tilde{M}(\tau)$ can be nonzero for $\tau = t - t' < 0$ and thus noncausal, where $\Delta\tilde{M}(\tau)$ for $\tau < 0$ is given by

$$\Delta\tilde{M}(\tau) = \int_{E_l}^{\infty} e^{iE'|\tau|}\,\Delta M(E')\,dE'. \tag{A2}$$

In k space, $\Delta\tilde{M}(\tau)$ becomes

$$\begin{aligned}\Delta\tilde{M}(\tau) &= \int_C \frac{1}{2i}\,e^{ik^2|\tau|}(e^{2ika}-1)dk\;\delta(r-a)\\ &= \int_C f(k)dk\;\delta(r-a),\end{aligned} \tag{A3}$$

where the curve C, shown in Fig. 3, is from $k = i\kappa_0$ to ∞, with $\kappa_0 \geq \sqrt{(\epsilon + B)}$, where ϵ is the energy of the one and only excited state in the model and B is the binding energy of the lowest bound state of the combined system of target and projectile (or zero, if there are no bound states). To find the value of $\Delta\tilde{M}(\tau)$, it is useful to have a closed curve such as that of Fig. 4, in which the lower section of path 3 is chosen to be a convenient horizontal line in the complex k plane, and the upper section is chosen to be along the $y = x$ line. Since the integrand in Eq. (A3) is an analytic function, the loop integral in k space is zero, which implies that

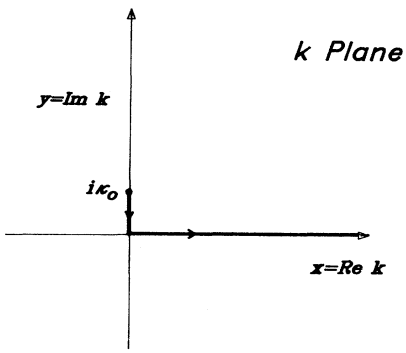

FIG. 3. The path of integration in Eq. (A2) transformed from the energy plane to the complex wave number plane in Eq. (A3).

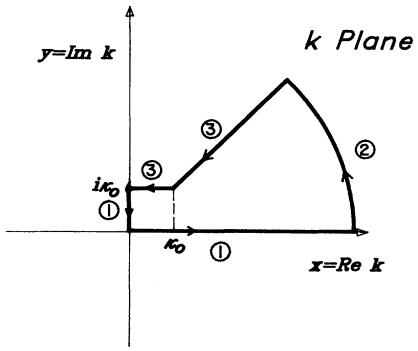

FIG. 4. The paths of integration used to demonstrate the noncausality of the potential of Appendix A.

$$\int_1 + \int_2 + \int_3 = 0. \tag{A4}$$

As the loop is extended to infinity, the integral along curve 2 approaches zero exponentially [4], which implies that

$$\int_1 = -\int_3 . \tag{A5}$$

Clearly, if the integral along 3 is nonzero, then the integral along 1 is nonzero as well and the potential is noncausal. Using the diagram of Fig. 4 for the path of integration, it is convenient to have k in the form $k = x + iy$; giving

$$f(k) = \frac{1}{2i}\,e^{-2xy|\tau|}e^{i(x^2-y^2)|\tau|}[e^{-2ya}e^{2ixa} - 1]. \tag{A6}$$

First, to show that the potential will be causal for the usual case, where the integration is carried out from $E = -\infty = k^2$, $(k = i\infty)$ to $E = \infty$, we take the limit as $y = \kappa_0 \to \infty$. With this limit, the first term in the bracket goes to zero and the first factor will dominate the expression giving an upper limit of

$$\lim_{y\to\infty}\int_0^y \frac{-1}{2i}\,e^{-2xy|\tau|}\,dx = \lim_{y\to\infty}\frac{1}{2i}\left(0 + \frac{1}{2y|\tau|}\right) = 0. \tag{A7}$$

So, as the lower limit to the energy integral goes to $-\infty$, the potential is causal, which is in agreement with [4] and with Titchmarsh's theorem.

Now for a finite lower limit $k_0 = i\kappa_0$, corresponding to an energy below the value $-\epsilon - B$ as in Fig. 3, the integral is of the form

$$\int_0^{\kappa_0} f(x + i\kappa_0)dx + \int_{\kappa_0}^{\infty} f(x + ix)dx. \tag{A8}$$

To show that the integral may be nonzero, consider values of a and κ_0 greater than or equal to unity and $|\tau|$ much greater than unity. Clearly the second integral in Eq. (A8) will be negligible due to the $e^{-2x^2|\tau|}$ factor in Eq. (A6) on the $y = x$ line, since $|\tau| \gg 1$.

In the remaining integral, the first term of Eq. (A8) is

$$\int_0^{\kappa_0} \frac{1}{2i} e^{-2x\kappa_0|\tau|} e^{i(x^2-\kappa_0^2)|\tau|} [e^{-2\kappa_0 a} e^{2ixa} - 1] dx. \quad \text{(A9)}$$

Evaluating these integrals numerically along path 3 for a typical value of a=5 and convenient values of $\kappa_0 = 1.0$ and $|\tau| = 25.0$ results in a value on the order of 10^{-20} for the term with the two exponential factors in the brackets and 10^{-2} for the -1 term; thus the two terms cannot cancel, so the integral is nonzero and the potential is noncausal.

APPENDIX B: ANALYTIC PROPERTIES OF THE RETARDED SELF-ENERGY

In this appendix we consider the analytic properties of N^R. We start by writing Dyson's Equation (36) as the matrix equation

$$G = G^0 + G^0(N - U)G, \quad \text{(B1)}$$

where each of these quantities is a matrix in discretized κ space. Multiplying Eq. (B1) on the left by $(G^0)^{-1}$ and on the right by $(G)^{-1}$ and solving for N gives the well known expression for the self-energy [5,6],

$$\begin{aligned} N &= U + (G^0)^{-1} - (G)^{-1} \\ &= U + (G_p^0 + G_h^0)^{-1} - (G_p + G_h)^{-1}. \end{aligned} \quad \text{(B2)}$$

Corresponding to G^R we define a retarded self-energy using Eq. (46),

$$\begin{aligned} N^R(\omega) &= U + [G_p^0(\omega) + G_h^{0\dagger}(\omega^*)]^{-1} \\ &\quad -[G_p(\omega) + G_h^{\dagger}(\omega^*)]^{-1} \\ &= U + [G^{0R}(\omega)]^{-1} - [G^R(\omega)]^{-1}. \end{aligned} \quad \text{(B3)}$$

For scattering energies N^R is identical to N, which justifies our use of the altered Dyson equation to treat the scattering problem.

Since N^R involves the inverses of the zero-order and exact Green's functions, it is important that we know the analytic properties of these inverses. Because of the defining relationship $(G^R)^{-1}G^R = 1$, if G^R is multiple valued, then its inverse must also be multiple valued in an exactly compensating way, so the product will be unity. If G^R has a simple pole at a point $\omega = \omega_0$, then each cofactor matrix of G^R will approach a constant times $(\omega - \omega_0)^{-(n-1)}$, where n is the number of rows of the matrix, and the determinant will approach $(\omega - \omega_0)^{-n}$. The inverse matrix of G^R will therefore approach $\omega - \omega_0$; that is, it will have a zero at the singular points of G^R. Poles of the $(G^R)^{-1}$ will occur at the zeros of G^R. All of these same statements also apply to the G^{0R}.

The change of sign in the η term of Eq. (43) in the hole Green's function of Eq. (46) shifts the singularities of G^R to the lower half ω plane (see Fig. 2). Because of the connection Eq. (B3), the singularities in N^R are also shifted to the lower half plane. Poles in G^R and G^{0R} become zero terms of N^R [Eq. (B3)] (which, of course, are not singularities), branch points and cuts of G^R become branch points and cuts of N^R, and zeros of G^R become poles of N^R. The fact that G^R is analytic in the upper half ω plane means that N^R is also analytic except for the possibility that the retarded Green's function might have a zero.

It is therefore important to determine whether G^R or G^{0R} can have a zero in the upper half plane. Luttinger has shown [13] for spinless Fermions in the absence of an external potential that $\mathrm{Im}\, G < 0$, that is, $\mathrm{Im}\, G$ is negative definite. The same argument applies to $\mathrm{Im}\, G^R$. Luttinger states [13] that this result also applies to the more general case, that is, G has no singularities in the upper half plane. We have verified this result by showing [14] that a matrix representation of G^R has a nonzero determinant, which implies that G^R has an inverse and therefore no singularities in the upper half plane.

At infinite values of ω, both G^R and G^{0R} approach zero as $1/\omega$, as described earlier in this appendix. Thus the inverse matrices in Eq. (B3) will each approach ω. They cancel in Eq. (B3), leaving at worst a constant at ∞. This is acceptable behavior in the limit as $|\omega| \to \infty$, since the exponential $e^{-i\omega\tau}$ in the Fourier integral Eq. (48) goes to zero exponentially at negative values of τ as $\mathrm{Im}\,\omega \to \infty$. Thus on an infinite semicircle in the upper-half ω plane, the product $N^R e^{-i\omega\tau}$ approaches zero rapidly enough that the contribution to the integral on the semicircle is zero for negative τ, a result needed in the proof of Titchmarsh's theorem. Since there are no singularities in the (finite) upper-half plane, Cauchy's theorem gives zero for Eq. (48) for negative τ, which is the causality condition. On the other hand, the self-energy N for the time-ordered Green's function G will not generally be causal because of the singularities in G_h in the upper half plane.

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