General formulation for direct evaluation of the local field amplitude and transition amplitude based on the Fredholm determinant

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We develop a determinantal method in a quantum scattering system for direct evaluation of various quantities including the local field amplitude and transition amplitude (*S*-matrix element). This method is applicable to multichannel elastic and inelastic scattering systems without rearranging the particles. The underlying principle of our formulation is that requested information can be extracted from a wave operator without solving the wave equation. The wave operator is the master operator maintaining all of the information about a system; the determinant of the inverse wave operator is just the Fredholm determinant. In the 1960s, a similar determinantal method was developed for the *S*-matrix element or equivalently the far-field amplitude of the wave function. Until now, however, no determinantal method for near-field quantities existed, although de Broglie and electromagnetic near fields are observable using scanning probe microscopes. Additionally, we prove that our formula for *S*-matrix element covers the known formula (the Le Couteur-Newton formula).

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I. INTRODUCTION

Prior to the 1980s, there was no clear way of investigating de Broglie and electromagnetic near fields because no method existed to observe them. All scattering experiments had been performed using far-field observations, and in view of scattering theory, the central role was played by the *S* matrix, which represents the transition amplitude and far-field amplitude simultaneously. It was Wheeler [1] who introduced the *S* matrix and evaluated it using the Fredholm determinant. He treated a nuclear collision problem and used the Fredholm determinant to assign a bound state. In Wheeler's scheme, one can calculate *S*-matrix elements directly without solving the wave equation and without knowing the near field. Following from this work, a systematic procedure was established. Le Couteur [2] expressed the elements of the *S* matrix in terms of a single function of channel wave numbers and derived a substitution rule. Newton [3,4] subsequently identified Le Couteur's function as just the Fredholm determinant in wave number representation.

During the 1980–1990s, various scanning probe microscopes were developed to observe de Broglie and electromagnetic near fields including the scanning tunneling microscope [5], atomic force microscope [6,7], and scanning near-field optical microscope [8,9]. The near fields are calculated theoretically by solving the Schrödinger equation and Maxwell's equations. In principle, however, effort expended on constructing a solution beyond the near-field region of interest is wasted, and in contrast to far-field theory, no determinantal method exists to evaluate near-field quantities. Recently, the enhancement of de Broglie and electromagnetic near fields has attracted great interest, such as in systems with nanocontacts [10,11] and local plasmons [12]. A determinantal (direct) method is desirable in such systems and will be useful to explore the optimal parameters to enhance the near-field amplitude at a desired position.

Here, we present a general determinantal formulation for direct evaluation of various quantities related to both near and far fields such as the local field amplitude and the *S*-matrix element. Our formulation is developed in the framework of formal scattering theory based on the principle that a desired quantity can be extracted directly from the wave operator, which is the master operator maintaining all of the information about the system. Using the Fredholm determinant and Cramer's rule, we derive determinantal formulas that are effective in multichannel elastic and inelastic scattering systems without rearrangement of particles. Our formula for *S*-matrix elements leads to the Le Couteur–Newton formula and both are effective in the space of open channels. It is still a remaining problem in the determinantal formulation to evaluate *S*-matrix elements related to closed channels.

There is another approach used to evaluate the matrix element directly: Green's function method [13]. This method is frequently applied to quantum many-body problems in the scheme of perturbation and renormalization and is not readily applicable to scattering systems in an exact numerical scheme.

The outline of this paper is as follows. In Sec. II, notations necessary for formal scattering theory are introduced. In Sec. III, determinantal formulas for the local field amplitude, transition amplitude (*S*-matrix element), etc. are derived on an equal footing. In Sec. IV, applications are demonstrated by numerical calculations of the local field amplitude in one- and three-dimensional elastic (potential) quantum scattering systems and by analytical calculations of the *S*-matrix element in one-dimensional elastic (potential) and inelastic scattering systems. In Sec. V, we prove that our formula covers the Le Couteur–Newton formula. We state our conclusions in Sec. VI and provide an outlook for future developments. Appendix A is needed for Sec. II. Appendix B gives analytical solutions of the problems described in Sec. IV. Appendix C contains lemmas and the current conservation law related to Sec. V.

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II. NOTATIONS

In this section, the notation required for the framework of formal scattering theory on a given energy shell is introduced. Suppose there are scattering fields $|k(\pm)\rangle$ satisfying the next Lippmann-Schwinger equation in abstract vector space,

$$|k(\pm)\rangle = |k\rangle + \hat{G}^{(0\pm)}\hat{V}|k(\pm)\rangle, \tag{1}$$

where $|k\rangle$ is the incident field with wave number k of the traveling particle, $\hat{V}$ is the scattering potential operator, and $\hat{G}^{(0+)}$ and $\hat{G}^{(0-)}$ are the retarded and advanced Green's operators, respectively, in a system without a scattering potential [14]. Although the retarded solution, $|k(+)\rangle$, satisfies causality and is physically acceptable, we also need the advanced (unphysical) solution, $|k(-)\rangle$, to construct the S matrix. The formulas in terms of k are easily extended to a system with any number of spatial dimensions and a field with internal degrees of freedom such as spinor, vector, and composite particles. In those cases, one should reconsider k as a set of adequate labels for channels including a wave number. Equation (1) is expressed in terms of the Fredholm integral operator $\hat{F}^{(\pm)}$,

$$\hat{F}^{(\pm)}|k(\pm)\rangle = |k\rangle, \tag{2}$$

$$\hat{F}^{(\pm)} \equiv (\hat{1} - \hat{G}^{(0\pm)}\hat{V}). \tag{3}$$

In contrast, a bound state $|B\rangle$ is a self-excited field without an incident field, so that the following equation is satisfied [15]:

$$\hat{F}^{(\pm)}|B\rangle = 0, \tag{4}$$

i.e.,

$$\det \hat{F}^{(\pm)} = 0. \tag{5}$$

Equations (2) and (4) indicate that the Fredholm integral operator $\hat{F}^{(\pm)}$ is the master operator determining all the solutions of Eq. (1).

From Eq. (5) it follows that the solutions of Eq. (1) contain at least one bound state in the domain. In practice, a bound state cannot coexist with scattering states in the same energy shell because an infinitesimal perturbation would destroy the bound state. Therefore, in this paper, the following condition is assumed:

$$\det \hat{F}^{(\pm)} \neq 0. \tag{6}$$

The wave operator $\hat{W}^{(\pm)}$ and source operator $\hat{M}^{(\pm)}$ are also master operators and defined by the following equations:

$$|k(\pm)\rangle = \hat{W}^{(\pm)}|k\rangle, \tag{7}$$

$$\hat{V}|k(\pm)\rangle = \hat{M}^{(\pm)}(\hat{V}|k\rangle). \tag{8}$$

Equations (7) and (8) indicate that the wave and source operators produce the true field and the true source from the field and the source in the lowest order Born approximation, respectively. The wave operator $\hat{W}^{(\pm)}$ was first introduced by Møller [16], and the source operator $\hat{M}^{(\pm)}$ is described in our previous paper [17].

The Fredholm determinant is defined as $\det \hat{F}^{(\pm)}$ and satisfies the following relationships under condition (6):

$$\det \hat{F}^{(\pm)} = 1/\det \hat{W}^{(\pm)} = 1/\det \hat{M}^{(\pm)}, \tag{9}$$

where the last equality was proved in Ref. [17].

In the entire space, the following conditions are assumed for normalization, orthogonality, and completeness [18,19]:

$$\langle k'|k\rangle = \delta(k'-k), \tag{10}$$

and

$$\langle k'(\pm)|k(\pm)\rangle = \delta(k'-k),$$

$$\langle B'|B\rangle = \delta_{B'B}, \tag{11}$$

$$\langle B|k(\pm)\rangle = \langle k(\pm)|B\rangle = 0,$$

and

$$\hat{1} = \int dk|k\rangle\langle k| = \int dk|k(\pm)\rangle\langle k(\pm)| + \sum_B |B\rangle\langle B|. \tag{12}$$

In Eq. (12), k runs over all the wave numbers belonging to on- and off-shell states, and if it exists, the inner degrees of freedom; B runs over all the bound states.

From Eqs. (11) and (12), Fredholm integral operator (2) and wave operator (7) on the E_k shell read

$$\hat{F}^{(\pm)} = \lim_{\Delta E_k \to 0} \int dk|k\rangle\langle k(\pm)|, \tag{13}$$

$$\hat{W}^{(\pm)} = \lim_{\Delta E_k \to 0} \int dk|k(\pm)\rangle\langle k|, \tag{14}$$

where ΔE_k is a small section including the shell energy E_k. Equations (13) and (14) lead to

$$\hat{F}^{(\pm)-1} = \hat{F}^{(\pm)\dagger} = \hat{W}^{(\pm)}, \tag{15}$$

$$\hat{W}^{(\pm)-1} = \hat{W}^{(\pm)\dagger} = \hat{F}^{(\pm)}, \tag{16}$$

where the superscript † is the Hermite conjugate.

In terms of the master operators, the scattering operator (S matrix) and transition operator (T matrix) are expressed as [20]

$$\hat{S} = \hat{W}^{(-)\dagger}\hat{W}^{(+)}, \tag{17}$$

$$\hat{T}^{(\pm)} = \hat{V}\hat{W}^{(\pm)} = \hat{M}^{(\pm)}\hat{V}. \tag{18}$$

The matrix elements of wave and S operators are

$$\langle k'|\hat{W}^{(\pm)}|k\rangle = \langle k'|k\rangle + \left[\mp i\pi\delta(E_k - E_{k'}) + \mathrm{P}\frac{1}{E_k - E_{k'}}\right] \times \langle k'|\hat{T}^{(\pm)}|k\rangle, \tag{19}$$

$$\langle k'|\hat{S}|k\rangle = \langle k'|k\rangle - 2\pi i\langle k'|\hat{T}^{(+)}|k\rangle\delta(E_{k'} - E_k), \tag{20}$$

where $|k\rangle$ and $|k'\rangle$ are the initial and final states with well-defined energies E_k and $E_{k'}$, respectively, and $|k'\rangle$ possibly has an off-shell energy, $E_{k'}(\neq E_k)$. P stands for the principal part as an integral kernel. Equation (19) is proved in Appendix A and Eq. (20) is found in Ref. [21].

In a given energy shell, the S-matrix element (20) has the divergent factor $\delta(E_{k'}-E_k)$ originating from energy conservation and it is convenient to define the on-shell S matrix, which has no singularity and directly relates to the far-field amplitude. For this purpose, k is decomposed into two parts, E_k and Ω_k; the former is the total energy as a function of k and the latter stands for all the other degrees of freedom such as solid angle, orbital and spin angular momentums, etc. The δ function and integral metric are expressed as

$$\langle k'|k\rangle = \delta(k'-k) = \delta(E_{k'} - E_k)\frac{1}{\mathcal{D}_{k'}}\delta(\Omega_{k'} - \Omega_k), \tag{21}$$

$$dk = \mathcal{D}_k dE_k d\Omega_k, \tag{22}$$

$$\mathcal{D}_k = \left|\frac{k_{\text{w.n.}}^{d-1}}{\nabla_{k_{\text{w.n.}}}E_k}\right|, \tag{23}$$

where $k_{\text{w.n.}}$ is the wave number included in the label k and d is the spatial dimension of the system. $\mathcal{D}_k$ means the density of states in the neighborhood of k. From Eqs. (19) and (20), the matrix element of the wave operator has the same type of singularity as the S-matrix element. Furthermore, the matrix element of the Fredholm integral operator has the same singularity due to Eq. (15) or Eq. (16). Therefore, the on-shell S, Fredholm integral, and wave operators can be defined implicitly through

$$\langle k'|\hat{A}|k\rangle = \langle k'|\hat{A}_{\text{on shell}}|k\rangle\delta(E_{k'} - E_k)\frac{1}{\mathcal{D}_{k'}} + (\text{finite value}),$$

$$\hat{A} = \hat{S}, \hat{S}^\dagger, \hat{F}^{(\pm)}, \hat{F}^{(\pm)\dagger}, \hat{W}^{(\pm)}, \hat{W}^{(\pm)\dagger}. \tag{24}$$

Note that Eq. (24) contains the density of final states, but not of initial states. In particular, the on-shell S-matrix element leads to the following expression using Eqs. (20) and (21):

$$\langle k'|\hat{S}_{\text{on shell}}|k\rangle = \delta(\Omega_{k'} - \Omega_k) - 2\pi i\mathcal{D}_{k'}\langle k'|\hat{T}^{(+)}|k\rangle. \tag{25}$$

The next relationship between the on-shell S and wave operators is derived from Eqs. (17), (22), and (24) ($\hat{A} = \hat{S}, \hat{W}^{(+)}, \hat{W}^{(-)\dagger}$):

$$\langle k'|\hat{S}_{\text{on shell}}|k\rangle = \int_{E_k\ \text{shell}} d\Omega_{k''}\langle k'|(\hat{W}^{(-)\dagger})_{\text{on shell}}|k''\rangle \times\langle k''|\hat{W}^{(+)}_{\text{on shell}}|k\rangle. \tag{26}$$

The inverse of the on-shell Fredholm integral and wave operators are defined by

$$\begin{aligned}&\int_{E_k\ \text{shell}} d\Omega_{k''}\langle k'|(\hat{A}_{\text{on shell}})^{-1}|k''\rangle\langle k''|\hat{A}_{\text{on shell}}|k\rangle \\ &= \int_{E_k\ \text{shell}} d\Omega_{k''}\langle k'|\hat{A}_{\text{on shell}}|k''\rangle\langle k''|(\hat{A}_{\text{on shell}})^{-1}|k\rangle \\ &= \delta(\Omega_{k'} - \Omega_k),\end{aligned}$$

$$\hat{A} = \hat{F}^{(\pm)}, \hat{W}^{(\pm)}. \tag{27}$$

From Eqs. (15), (16), (21), and (24), we may identify the inverse on-shell operators as

$$(\hat{F}^{(\pm)}_{\text{on shell}})^{-1} = (\hat{F}^{(\pm)\dagger})_{\text{on shell}} = \hat{W}^{(\pm)}_{\text{on shell}}, \tag{28}$$

$$(\hat{W}^{(\pm)}_{\text{on shell}})^{-1} = (\hat{W}^{(\pm)\dagger})_{\text{on shell}} = \hat{F}^{(\pm)}_{\text{on shell}}. \tag{29}$$

Note that, for example, $(\hat{F}^{(\pm)\dagger})_{\text{on shell}} \neq (\hat{F}^{(\pm)}_{\text{on shell}})^\dagger$ because of definition (24).

III. DETERMINANTAL FORMULATION FOR VARIOUS QUANTITIES

In this section, we prove the determinantal formulas in a unified manner for the local field amplitude and the transition amplitude (S-matrix element and T-matrix element). As in the previous section, the formulas presented here are easily extended to spinor or vector fields in arbitrary dimensional space. All the determinantal formulas are derived from the following two lemmas, which are essentially Cramer's rule [22] for the solution X_i of linear simultaneous equations $\Sigma_{i=0}^N X_i A_{ij} = B_j$ and $\Sigma_{j=0}^N A_{ij} X_j = B_i$ with $\det A \neq 0$ [23]:

$$\begin{aligned}\sum_i B_i(A^{-1})_{ij} &= \frac{\det A_{[j\bullet\to B_\bullet]}}{\det A} \\ &= \frac{1}{\det A}\det\begin{bmatrix} A_{00} & \cdots & A_{0k} & \cdots & A_{0N} \\ \vdots & & \vdots & & \vdots \\ A_{j-10} & \cdots & A_{j-1k} & \cdots & A_{j-1N} \\ B_0 & \cdots & B_k & \cdots & B_N \\ A_{j+10} & \cdots & A_{j+1k} & \cdots & A_{j+1N} \\ \vdots & & \vdots & & \vdots \\ A_{N0} & \cdots & A_{Nk} & \cdots & A_{NN} \end{bmatrix},\end{aligned} \tag{30}$$

$$\sum_j (A^{-1})_{ij}B_j = \frac{\det A_{[\bullet i\to B_\bullet]}}{\det A}, \tag{31}$$

where $A_{[j\bullet\to B_\bullet]}$ in Eq. (30) and $A_{[\bullet i\to B_\bullet]}$ in Eq. (31) are modified matrices of A; the jth row vector of A is replaced by vector B^t in the former, while the ith column vector is replaced by the vector B in the latter. In the following, we assume that the solutions of Eq. (1) on a given energy shell do not contain a bound state, i.e., condition (6). Furthermore, an operator is considered as a matrix with continuous indices, and lemmas (30) and (31) are applied.

The local field amplitude is expressed in terms of the Fredholm determinant and evaluated as follows:

$$\langle x|k(+)\rangle = \langle x|\hat{W}^{(+)}|k\rangle = \int dx' \langle x|\hat{W}^{(+)}|x'\rangle\langle x'|k\rangle \tag{32}$$

$$= \frac{\det(\hat{W}^{(+)-1})_{[\bullet x \to \langle \bullet|k\rangle]}}{\det(\hat{W}^{(+)-1})} = \frac{\det(\hat{F}^{(+)})_{[\bullet x \to \langle \bullet|k\rangle]}}{\det \hat{F}^{(+)}}. \tag{33}$$

From Eq. (32) to Eq. (33), we use lemma (31) with Eq. (16). Note that Eq. (33) is effective for both near- and far-field amplitudes.

In the same manner, the determinantal formula for the on-shell S-matrix element is derived from Eqs. (26), (29), and (30),

$$\begin{aligned}\langle k'|\hat{S}_{\text{on shell}}|k\rangle &= \frac{\det(\hat{W}^{(+)}_{\text{on shell}})^{-1}_{[k\bullet \to \langle k'|(\hat{W}^{(-)\dagger})_{\text{on shell}}|\bullet\rangle]}}{\det(\hat{W}^{(+)}_{\text{on shell}})^{-1}} \\ &= \frac{\det(\hat{W}^{(+)}_{\text{on shell}})^{-1}_{[k\bullet \to \langle k'|(\hat{W}^{(-)}_{\text{on shell}})^{-1}|\bullet\rangle]}}{\det(\hat{W}^{(+)}_{\text{on shell}})^{-1}} \\ &= \frac{\det(\hat{F}^{(+)}_{\text{on shell}})_{[k\bullet \to \langle k'|\hat{F}^{(-)}_{\text{on shell}}|\bullet\rangle]}}{\det \hat{F}^{(+)}_{\text{on shell}}}.\end{aligned} \tag{34}$$

One can evaluate Eq. (34), as far as we can construct $\hat{G}^{(0\pm)}$ in Eq. (3). The present formulas are effective for evaluating matrix elements in the space of open channels because the basis set is assumed to have real wave numbers. Equation (34) not only covers the Le Couteur–Newton formula (see Sec. V) but also has extended applicability to various systems (see Secs. IV C and IV D).

In the same manner, one can derive determinantal formulas for various quantities such as the local scattering potential amplitude $\langle x|\hat{V}|k(+)\rangle = \langle x|\hat{M}^{(+)}\hat{V}|k\rangle$, the local current density $\langle x|\hat{p}|k(+)\rangle = \langle x|\hat{p}\hat{W}^{(+)}|k\rangle$ (where $\hat{p}$ is the momentum operator), and the T-matrix element $\langle k'|\hat{T}^{(+)}|k\rangle$ with Eq. (18). The determinantal formulas for these quantities are as follows:

$$\langle x|\hat{V}|k(+)\rangle = \int dx' \langle x|\hat{M}^{(+)}|x'\rangle\langle x'|\hat{V}|k\rangle$$

$$= \frac{\det(\hat{M}^{(+)-1})_{[\bullet x \to \langle \bullet|\hat{V}|k\rangle]}}{\det(\hat{M}^{(+)-1})}, \tag{35}$$

$$\langle x|\hat{p}|k(+)\rangle = \frac{\det(\hat{W}^{(+)-1})_{[k\bullet \to \langle x|\hat{p}|\bullet\rangle]}}{\det(\hat{W}^{(+)-1})} = \frac{\det(\hat{F}^{(+)})_{[k\bullet \to \langle x|\hat{p}|\bullet\rangle]}}{\det \hat{F}^{(+)}}, \tag{36}$$

$$\langle k'|\hat{T}^{(+)}|k\rangle = \frac{\det(\hat{M}^{(+)-1})_{[\bullet k' \to \langle \bullet|\hat{V}|k\rangle]}}{\det(\hat{M}^{(+)-1})} \tag{37}$$

$$= \frac{\det(\hat{W}^{(+)-1})_{[k\bullet \to \langle k'|\hat{V}|\bullet\rangle]}}{\det(\hat{W}^{(+)-1})} = \frac{\det(\hat{F}^{(+)})_{[k\bullet \to \langle k'|\hat{V}|\bullet\rangle]}}{\det \hat{F}^{(+)}}. \tag{38}$$

The above formulas represent a generalization of our previous work [17,24], in which we formulated the transition amplitude in a one-dimensional potential scattering system. In Eq. (33) and Eqs. (35)–(38), the basis set to construct the matrix elements should be complete over the entire space. Indeed, all of the k states on and off the energy shell are needed to calculate Eqs. (36)–(38). This is because B in lemmas (30) and (31) has no singularity, so that its contractions with on-shell elements (singular minority) and off-shell elements (nonsingular majority) of A contribute to the same order. This situation is different from that of the S-matrix element; both B and A in Eq. (17) have the on-shell singularities [see Eq. (19)], which dominate the contraction.

IV. APPLICATIONS

In Secs. IV A and IV B of this section, we demonstrate numerical calculations of the local field amplitude in both one- and three-dimensional elastic (potential) scattering systems, respectively. Section IV A aims to explain the procedure used for the numerical calculations, and Sec. IV B emphasizes the applicability of our formula to real systems. Furthermore, analytical calculations of on-shell S-matrix elements are performed in multichannel elastic and inelastic scattering systems in Secs. IV C and IV D, respectively.

A. Local field amplitude in a one-dimensional potential scattering system

Here, we test determinantal formula (33) for the local field amplitude in a simplified system and explain the procedure used for the numerical calculations. Suppose that a scalar field satisfies the one-dimensional Schrödinger equation with a static scattering potential, as shown in Fig. 1,

$$(-\partial_x^2 - k^2)\langle x|k(+)\rangle = -V(x)\langle x|k(+)\rangle. \tag{39}$$

Schrödinger equation (39) can be rewritten in integral form, Eq. (1), in abstract vector space. Then, in the coordinate representation, the quantities appearing in Eq. (39) or Eq. (1) read

$$\langle x|k\rangle = \frac{e^{ikx}}{\sqrt{2\pi}} \quad \text{or} \quad \langle k|x\rangle = \frac{e^{-ikx}}{\sqrt{2\pi}}, \tag{40}$$

$$\langle x|\hat{V}|x'\rangle = V(x)\delta(x-x'), \tag{41}$$

$$\langle x|\hat{G}^{(0+)}|x'\rangle = G^{(0+)}(x,x') = \frac{e^{ik|x-x'|}}{2ik}, \tag{42}$$

where k is real and $k>0$. The Green's function satisfies the following equation and the outgoing scattering boundary condition:

$$(-\partial_x^2 - k^2)G^{(0+)}(x,x') = -\delta(x-x'). \tag{43}$$

Furthermore, from Eq. (3), the Fredholm integral (inverse wave) operator is easily expressed in the coordinate representation as

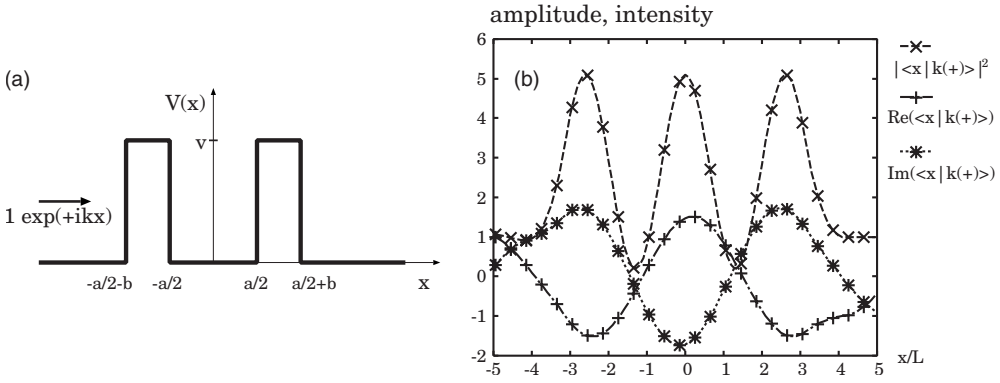

FIG. 1. (a) One-dimensional potential scattering system with $k=1.204L^{-1}$, $a=2\pi L$, $b=1L$, $v=2L^{-2}$, and $k\Delta x=0.05$, where L is arbitrary unit of length. (b) Numerical calculations based on the determinantal formula (discrete points) and analytical calculations (lines) for the system shown in (a). An incident plane wave with unit amplitude originates from the left-hand side region.

$$F^{(+)}(x,x') = \langle x|\hat{F}^{(+)}|x'\rangle = \langle x|\hat{W}^{(+)-1}|x'\rangle = \delta(x-x') - G^{(0+)}(x,x')V(x'). \tag{44}$$

First, in order to obtain a matrix representation of Fredholm integral operator (3), the infinite domain of x is approximated by the finite domain $[x_l-\Delta x/2, x_u+\Delta x/2]$, where x_l and x_u are large negative and positive values, respectively, and $\Delta x=(x_u-x_l)/N$; N is set to be a sufficiently large number so that $k\Delta x \ll 1$ is satisfied. Now we can define an ith window function $(i=0,1,\ldots,N)$ as

$$\langle x|i\rangle = \frac{\theta[x-(x_i-\Delta x/2)]\theta[(x_i+\Delta x/2)-x]}{\sqrt{\Delta x}}, \tag{45}$$

where

$$\theta(x) = \begin{cases} 1 & \text{for } x>0 \\ \frac{1}{2} & \text{for } x=0 \\ 0 & \text{for } x<0, \end{cases}$$

and

$$x_i = x_l + i\Delta x.$$

The basis set of the window functions is normalized, orthogonal, and is assumed to be complete, i.e.,

$$\langle i|j\rangle = \delta_{ij}, \quad \sum_{i=0}^{N} |i\rangle\langle i| = \hat{1}. \tag{46}$$

Then, the matrix element corresponding to Eq. (44) becomes

$$F_{ij}^{(+)} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx' \langle i|x\rangle F^{(+)}(x,x')\langle x'|j\rangle \simeq \delta_{ij} - G^{(0+)}(x_i,x_j)V(x_j)\Delta x. \tag{47}$$

Next, a modification must be considered to evaluate the numerator in Eq. (33). Suppose that the observation point x belongs to the pth section [i.e., $\langle x|p\rangle \neq 0$ in the meaning of Eq. (45)]. The coordinate x is approximated by x_p that is the representative point of pth section. Then the pth column vector of matrix (47) is replaced by a column vector in which the ith component is evaluated from the incident field as

$$\langle i|k\rangle = \int_{-\infty}^{+\infty} dx' \langle i|x'\rangle\langle x'|k\rangle = e^{ikx_i}\sqrt{\frac{\Delta x}{2\pi}}, \quad (i=0,1,\ldots,N). \tag{48}$$

Given the incidence with unit amplitude $\sqrt{2\pi}\langle x|k\rangle = e^{ikx}$, the local field amplitude at observation point x_p, $\sqrt{2\pi}\langle x_p|k(+)\rangle$, can be expressed using $(N+1)\times(N+1)$ matrices in the discrete coordinate representation:

$$\sqrt{2\pi}\langle x_p|k(+)\rangle = \sqrt{2\pi}\sum_i \langle x_p|i\rangle\langle i|k(+)\rangle = \sqrt{2\pi}\langle x_p|p\rangle\langle p|k(+)\rangle = \sqrt{\frac{2\pi}{\Delta x}}\frac{\det \hat{F}^{(+)}_{[\bullet p\to\langle\bullet|k\rangle]}}{\det \hat{F}^{(+)}} = \frac{\det\begin{bmatrix} F_{00}^{(+)} & \cdots & e^{ikx_0} & \cdots & F_{0N}^{(+)} \\ F_{10}^{(+)} & \cdots & e^{ikx_1} & \cdots & F_{1N}^{(+)} \\ \vdots & & \vdots & & \vdots \\ F_{N0}^{(+)} & \cdots & e^{ikx_N} & \cdots & F_{NN}^{(+)} \end{bmatrix}}{\det\begin{bmatrix} F_{00}^{(+)} & \cdots & F_{0p}^{(+)} & \cdots & F_{0N}^{(+)} \\ F_{10}^{(+)} & \cdots & F_{1p}^{(+)} & \cdots & F_{1N}^{(+)} \\ \vdots & & \vdots & & \vdots \\ F_{N0}^{(+)} & \cdots & F_{Np}^{(+)} & \cdots & F_{NN}^{(+)} \end{bmatrix}}. \tag{49}$$

Now, suppose $V(x_i)=0$ for a certain $i(\neq p)$. Then, one can expand $\det \hat{F}^{(+)}$ in a series of ith column vector elements $F_{ki}^{(+)}=\delta_{ki}(k=0,1,\ldots,N)$, and we find that the determinant in the denominator of Eq. (49) leads to $\widetilde{F^{(+)}}_{ii}$, which is the determinant of a $N\times N$ matrix of the cofactor of $F_{ii}^{(+)}$. The determinant in the numerator of Eq. (49) is treated in the same manner. Therefore, any row and column vector with null potential $[V(x_i)=0(i\neq p)]$ in the two determinants can be eliminated at the start of the calculations. In other words, we can restrict the domain of x to the region $\{x|V(x)\neq 0\}$ so that the calculations are simplified remarkably. Finally, we

obtain the determinantal formula for the observation point $x_p \in \{x|V(x)=0\}$:

$$\sqrt{2\pi}\langle x_p|k(+)\rangle = \frac{\det\begin{bmatrix} F_{00}^{(+)} & \cdots & F_{0M}^{(+)} & e^{ikx_0} \\ \vdots & & \vdots & \vdots \\ F_{M0}^{(+)} & \cdots & F_{MM}^{(+)} & e^{ikx_M} \\ F_{p0}^{(+)} & \cdots & F_{pM}^{(+)} & e^{ikx_p} \end{bmatrix}}{\det\begin{bmatrix} F_{00}^{(+)} & \cdots & F_{0M}^{(+)} \\ \vdots & & \vdots \\ F_{M0}^{(+)} & \cdots & F_{MM}^{(+)} \end{bmatrix}}, \quad (50)$$

and for $x_p \in \{x|V(x)\neq 0\}$:

$$\sqrt{2\pi}\langle x_p|k(+)\rangle = \frac{\det\begin{bmatrix} F_{00}^{(+)} & \cdots & e^{ikx_0} & \cdots & F_{0M}^{(+)} \\ \vdots & & \vdots & & \vdots \\ F_{M0}^{(+)} & \cdots & e^{ikx_M} & \cdots & F_{MM}^{(+)} \end{bmatrix}}{\det\begin{bmatrix} F_{00}^{(+)} & \cdots & F_{0p}^{(+)} & \cdots & F_{0M}^{(+)} \\ \vdots & & \vdots & & \vdots \\ F_{M0}^{(+)} & \cdots & F_{Mp}^{(+)} & \cdots & F_{MM}^{(+)} \end{bmatrix}}, \quad (51)$$

where $(M+1)$ is the number of sampling points in the region $\{x|V(x)\neq 0\}$ and determines the reduced size of the matrices. For the observation point $x_p \in \{x|V(x)\neq 0\}$, we can practically use Eq. (50) instead of Eq. (51), keeping $F_{ip}^{(+)}$ without replacement to e^{ikx_i}. This treatment might introduce a numerical error, but it decreases as $k\Delta x$ becomes small.

The above procedure is analogous to that for the transition amplitude in [17,24]. The numerical calculations for the system with $V(x_j)=v$ for $x_j \in \{x|V(x)\neq 0\}$ based on Eq. (50) are shown in Fig. 1; these results support our determinantal formula. Note that Fig. 1 reveals that there is no serious error in the region $x_p \in \{x|V(x)\neq 0\}$, where we use Eq. (50) instead of Eq. (51).

B. Local field amplitude in a three-dimensional potential scattering system

To demonstrate the applicability of our formula to a real system, we treat a three-dimensional potential scattering system. The numerical procedure developed for a one-dimensional system in the previous section can easily be extended to a three-dimensional system with adequate modifications, e.g.,

$$(42) \rightarrow \langle \mathbf{x}|\hat{G}^{(0+)}|\mathbf{x}'\rangle = G^{(0+)}(\mathbf{x},\mathbf{x}') = \frac{-1}{4\pi}\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}, \quad (52)$$

$$(45) \rightarrow \langle \mathbf{x}|i\rangle = \prod_{\alpha=0}^{2} \frac{\theta([\mathbf{x}-(\mathbf{x}_i-\Delta\mathbf{x}/2)]_\alpha)\,\theta([(\mathbf{x}_i+\Delta\mathbf{x}/2)-\mathbf{x}]_\alpha)}{\sqrt{(\Delta\mathbf{x})_\alpha}}, \quad (53)$$

$$(48) \rightarrow \langle i|\mathbf{k}\rangle = \int d^3x'\langle i|\mathbf{x}'\rangle\langle \mathbf{x}'|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{x}_i}\prod_{\alpha=0}^{2}\sqrt{\frac{(\Delta\mathbf{x})_\alpha}{2\pi}} \quad (i=0,1,\ldots,N), \quad (54)$$

where $\mathbf{x}_i$ is the position vector of the center of an ith small rectangular, for which the edge lengths are $(\Delta\mathbf{x})_\alpha, (\alpha=0,1,2)$.

The numerical procedure based on Eq. (50) in three dimensions is applicable to systems with a scattering potential of an arbitrary shape. To evaluate matrix elements in Eq. (50) [or Eq. (47)] in three dimensions, we employ the following equation to reduce the numerical error arising from the singularity of the Green's function for small values of $|\mathbf{x}_i-\mathbf{x}_j|$:

$$\begin{aligned} F_{ij}^{(+)} &= \delta_{ij} - \prod_{\alpha=0}^{2}\left(\int_{(\mathbf{x}_j-\Delta\mathbf{x}/2)_\alpha}^{(\mathbf{x}_j+\Delta\mathbf{x}/2)_\alpha} dX_\alpha\right) G^{(0+)}(\mathbf{x}_i,\mathbf{X})V(\mathbf{X}) \\ &\simeq \delta_{ij} - \left\{\prod_{\alpha=0}^{2}\left(\int_{(\mathbf{x}_j-\Delta\mathbf{x}/2)_\alpha}^{(\mathbf{x}_j+\Delta\mathbf{x}/2)_\alpha} dX_\alpha\right)\frac{1}{|\mathbf{x}_i-\mathbf{X}|}\right\} \\ &\quad \times \frac{-1}{4\pi}e^{ik|\mathbf{x}_i-\mathbf{x}_j|}V(\mathbf{x}_j). \end{aligned} \quad (55)$$

The integral in Eq. (55) can be analytically calculated using the following indefinite integral:

$$\begin{aligned} &\int dR_2\int dR_1\int dR_0\frac{1}{R} \\ &= \left\{R_1R_2\ln|R+R_0| + R_0^2\tan^{-1}\frac{R+R_1+R_2}{R_0}\right\} \\ &\quad + \{(0,1,2)\rightarrow(1,2,0)\} + \{(0,1,2)\rightarrow(2,0,1)\}, \end{aligned} \quad (56)$$

where $R=(R_0^2+R_1^2+R_2^2)^{1/2}$, and $\{(0,1,2)\rightarrow(1,2,0)\}$ and $\{(0,1,2)\rightarrow(2,0,1)\}$ are the terms from the first term in the right-hand side after permutation of the indices. There are various representations for the integral constant, which is not included in Eq. (56).

We now examine the system with homogeneous spherical scatterer with the radius a, $V(\mathbf{x})=v\,\theta(a-|\mathbf{x}|)$, although our formula and computational code is applicable to the scattering potential with arbitrary shape and distribution. The numerical results are compared with the analytical solution in Fig. 2; this again supports our determinantal formula and reveals applicability to realistic systems.

C. *S*-matrix element in a simplified multichannel elastic scattering system

Here, we examine the new formula for the on-shell *S*-matrix element, Eq. (34), in an analytical manner, applying it to a simple one-dimensional elastic (potential) scattering system. Suppose we have a one-dimensional elastic (potential) scattering system described by Eq. (39) with the incident field $\langle x|k\rangle$ and the scattering potential,

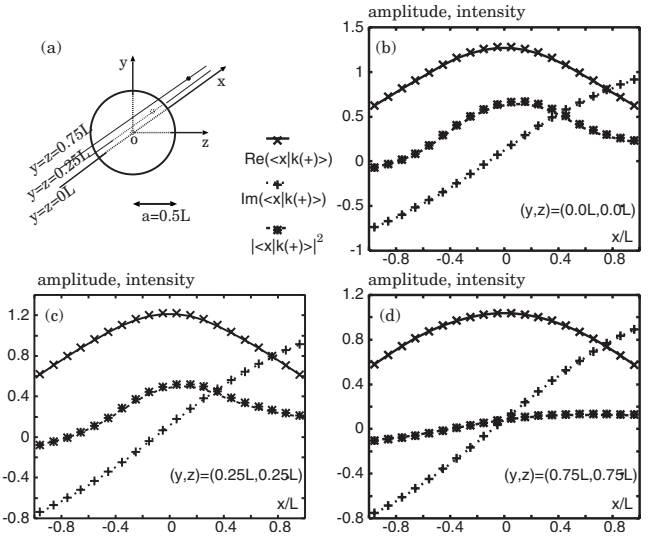

FIG. 2. (a) Spherical potential scattering system with $k=1L^{-1}$ $a=0.5L$, $v=-2L^{-2}$ (L is arbitrary unit of length), and $k(\Delta\mathbf{x})_\alpha=0.1$ for $\alpha=0,1,2$. The sphere is approximated by a stack of 552 small cubes with edges of $k(\Delta\mathbf{x})_\alpha$ in dimensionless length. The incident plane wave with unit amplitude propagates in the $+x$ direction. (b) Numerical calculations based on the determinantal formula (discrete points) and analytical calculations (lines) on the line $(y,z)=(0.00L,0.00L)$. [(c) and (d)] Same as (b), but on the line $(y,z)=(0.25L,0.25L)$ and $(y,z)=(0.75L,0.75L)$, respectively.

$$V(x)=v\,\delta(x). \tag{57}$$

This system is a two-channel elastic scattering system on a given energy shell [25]. Therefore, the asymptotic form of $\langle x|k(+)\rangle$ is expanded by the two basis functions on the energy shell, i.e., $\langle x|k\rangle$ and $\langle x|-k\rangle$. Using these two basis functions, the on-shell Fredholm integral (inverse wave) operator and S operator are expressed as 2×2 matrices. The matrix element of the (original) Fredholm integral operator between the initial and final states specified by $k_1,k_2\in\{+k,-k\}$ is

$$\begin{aligned}\langle k_2|\hat{F}^{(\pm)}|k_1\rangle &= \langle k_2|\hat{W}^{(\pm)-1}|k_1\rangle \\ &= \langle k_2|\hat{1}-\hat{G}^{(0\pm)}\hat{V}|k_1\rangle \\ &= \delta(k_2-k_1)-\int_{-\infty}^{+\infty}dx\frac{e^{-ik_2x\pm ik|x|}}{2(\pm i)k}\frac{v}{2\pi} \\ &= \delta(k_2-k_1)\pm iu[\delta(k_2+k)+\delta(k_2-k)] \\ &\quad +(\text{finite value}),\end{aligned} \tag{58}$$

$$u\equiv\frac{v}{4k}. \tag{59}$$

From Eqs. (21) and (23), the δ functions in Eq. (58) can be expressed in terms of energy, e.g., $\delta(k_2-k_1)=\delta(E_{k_2}-E_{k_1})/\mathcal{D}_{k_2}$, where $E_k=k^2$ and $\mathcal{D}_k=1/(2k)$. Comparing with Eq. (24) ($\hat{A}=\hat{F}^{(\pm)}$), one obtains the matrix representation of the on-shell Fredholm integral (inverse wave) operator as follows:

$$F^{(\pm)}_{\text{on shell}}=(W^{(\pm)}_{\text{on shell}})^{-1}=\begin{bmatrix}1\pm iu & \pm iu\\ \pm iu & 1\pm iu\end{bmatrix}, \tag{60}$$

where the basis function in the row and column is in the order of $|k\rangle,|-k\rangle$. The determinant is obtained by straightforward calculations:

$$\det\hat{F}^{(\pm)}_{\text{on shell}}=\det(\hat{W}^{(\pm)}_{\text{on shell}})^{-1}=1\pm 2iu. \tag{61}$$

Then, the on-shell S-matrix element is evaluated by Eq. (34) as

$$\langle k_2|\hat{S}_{\text{on shell}}|k_1\rangle=\frac{\det(\hat{F}^{(+)}_{\text{on shell}})_{[k_1\bullet\to\langle k_2|\hat{F}^{(-)}_{\text{on shell}}|\bullet\rangle]}}{\det\hat{F}^{(+)}_{\text{on shell}}}. \tag{62}$$

As a result, one can construct the on-shell S matrix,

$$S_{\text{on shell}}=\frac{1}{1+2iu}\begin{bmatrix}1 & -2iu\\ -2iu & 1\end{bmatrix}. \tag{63}$$

Equation (63) coincides with the far-field amplitude calculated analytically in Appendix B 1. Therefore, we ensure that our formula for on-shell S-matrix element is reasonable.

D. *S*-matrix element in a simplified multichannel inelastic scattering system

Here we test the new formula for the on-shell S matrix (34) in a simplified two-particle inelastic scattering system. Suppose we have a one-dimensional scattering system. A target scatterer at the origin possesses two internal energy levels, which can be excited or relaxed by a traveling particle. The Le Couteur–Newton formula is not applicable to this system because their formula is derived for a three-dimensional system in spherical coordinates. The model Hamiltonian $\hat{H}$ is composed of a null-interaction Hamiltonian $\hat{H}^{(0)}$ and the interaction potential operator $\hat{V}$ defined as follows:

$$\hat{H}=\hat{H}^{(0)}+\hat{V}, \tag{64}$$

$$\hat{H}^{(0)}=\int_{-\infty}^{+\infty}dx\frac{1}{-i}\partial_x\hat{\psi}^\dagger(x)\frac{1}{i}\partial_x\hat{\psi}(x)+\sum_{\zeta=0}^{1}\epsilon_\zeta\hat{b}_\zeta^\dagger\hat{b}_\zeta \tag{65}$$

$$=\int_{-\infty}^{+\infty}dkk^2\hat{a}^\dagger(k)\hat{a}(k)+\sum_{\zeta=0}^{1}\epsilon_\zeta\hat{b}_\zeta^\dagger\hat{b}_\zeta, \tag{66}$$

$$\hat{V}=\int_{-\infty}^{+\infty}dx\hat{\psi}^\dagger(x)[v\,\delta(x)\hat{b}_1^\dagger\hat{b}_0+v^*\delta(x)\hat{b}_0^\dagger\hat{b}_1]\hat{\psi}(x) \tag{67}$$

$$=\frac{1}{2\pi}(v\hat{b}_1^\dagger\hat{b}_0+v^*\hat{b}_1^\dagger\hat{b}_1)\int_{-\infty}^{+\infty}dk\int_{-\infty}^{+\infty}dk'\hat{a}^\dagger(k')\hat{a}(k), \tag{68}$$

where $\hat{\psi}^\dagger(x)$, $\hat{\psi}(x)$, and $\hat{b}_\zeta^\dagger,\hat{b}_\zeta$ are the creation and annihilation operators for the traveling particle and the target scat-

terer with internal state ζ, respectively; ϵ_ζ is the internal energy of the ζth level; v determines the strength of the interaction; and $\hat{a}^\dagger(k)$ and $\hat{a}(k)$ are the Fourier representations of $\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$, respectively:

$$\hat{\psi}(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dk e^{ikx}\hat{a}(k), \quad \hat{\psi}^\dagger(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dk e^{-ikx}\hat{a}^\dagger(k). \tag{69}$$

We may use the commutation relationship for either bosons or fermions; the commutation relationship does not affect the result because we assume there is one of each type of particle so that the quantum many-body problem is avoided:

$$[\hat{\psi}(x), \hat{\psi}^\dagger(x')]_\mp = \delta(x - x'), \tag{70}$$

$$[\hat{b}_\zeta, \hat{b}^\dagger_{\zeta'}]_\mp = \delta_{\zeta\zeta'}, \tag{71}$$

where $[\ ,\ ]_-$ and $[\ ,\ ]_+$ are the commutation relationships for bosons and fermions, respectively. We assume that other commutation relationships between $\hat{\psi}(x)s$ and $\hat{b}_\zeta s$ are zero, e.g., $[\hat{\psi}(x), \hat{b}^\dagger_\zeta]_- = 0$.

In the first step of the direct evaluation of the on-shell S-matrix element using the new formula (34), we calculate the free Green's function on the shell of total energy E:

$$\langle x\sigma|\hat{G}^{(0\pm)}|x'\sigma'\rangle = \sum_{\zeta=0}^{1} \frac{1}{\pm 2ik_\zeta} e^{\pm ik_\zeta|x-x'|} Z_\zeta(\sigma)\{Z_\zeta(\sigma')\}^*. \tag{72}$$

where $k_\zeta \equiv (E - \epsilon_\zeta + i0)^{1/2}$ in the double-value function, and one should take the branch where $k_\zeta > 0$ assuming the channel is open (i.e., k_ζ is a real). For the derivation of Eq. (72), we use the following calculations and notations:

$$\begin{aligned}\langle x|\hat{a}^\dagger(k)|0\rangle_{\text{spatial}} &= \langle x|k\rangle_{\text{spatial}} = \langle 0|\hat{\psi}(x)\hat{a}^\dagger(k)|0\rangle_{\text{spatial}} \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dk' e^{ik'x}\langle 0|\hat{a}(k')\hat{a}^\dagger(k)|0\rangle_{\text{spatial}} \\ &= \frac{1}{\sqrt{2\pi}}\exp(ikx),\end{aligned} \tag{73}$$

$$\langle\sigma|\hat{b}^\dagger_\zeta|0\rangle_{\text{internal}} = Z_\zeta(\sigma), \tag{74}$$

where $\langle\ |\ \rangle_{\text{spatial}}$ and $\langle\ |\ \rangle_{\text{internal}}$ indicate the inner products in the subspaces of the spatial and internal degrees of freedom, respectively. In Eq. (73), we use $[\hat{a}(k'), \hat{a}^\dagger(k)]_\mp = \delta(k' - k)$, which is derived from Eqs. (69) and (70).

Next, one may calculate 4×4 matrix representations of the Fredholm integral (inverse wave) operator on the energy shell. The bases are the four open channel functions with energy E, $\{|\pm k_\zeta\zeta\rangle\,|\,\zeta = 0, 1\}$. For example,

$$\begin{aligned}\langle k_{\zeta'}\zeta'|\hat{F}^{(\pm)}|k_\zeta\zeta\rangle &= \langle k_{\zeta'}\zeta'|\hat{W}^{(\pm)-1}|k_\zeta\zeta\rangle \\ &= \langle k_{\zeta'}\zeta'|\hat{1} - \hat{G}^{(0\pm)}\hat{V}|k_\zeta\zeta\rangle \\ &= \delta(k_{\zeta'} - k_\zeta)\delta_{\zeta\zeta'} - \int_{-\infty}^{+\infty} dx \frac{e^{-ik_{\zeta'}x \pm ik_\zeta|x|}}{2(\pm i)k_\zeta} \\ &\quad \times \frac{1}{2\pi}(v\delta_{\zeta'1}\delta_{\zeta 0} + v^*\delta_{\zeta'0}\delta_{\zeta 1}) \\ &= \delta(k_{\zeta'} - k_\zeta)\delta_{\zeta\zeta'} \pm i\delta(k_{\zeta'} - k_{\zeta'})(\delta_{\zeta'1}\delta_{\zeta 0}u_1 \\ &\quad + \delta_{\zeta'0}\delta_{\zeta 1}u_0) + (\text{finite value}),\end{aligned} \tag{75}$$

$$u_0 \equiv \frac{v^*}{4k_0}, \quad u_1 \equiv \frac{v}{4k_1}. \tag{76}$$

Other types of matrix elements are obtained by replacing $k_{\zeta'} \to -k_{\zeta'}$ and/or $k_\zeta \to -k_\zeta$ in Eq. (75). From Eqs. (21) and (23), the δ functions in Eq. (75) can be expressed in terms of energy, e.g., $\delta(k_{\zeta'} - k_\zeta)\delta_{\zeta'\zeta} = \delta(E_{k_{\zeta'}} - E_{k_\zeta})\delta_{\zeta'\zeta}/\mathcal{D}_{k_{\zeta'}}$, where $E_{k_\zeta} = \epsilon_\zeta + k_\zeta^2$ and $\mathcal{D}_{k_\zeta} = 1/(2k_\zeta)$. Comparing with Eq. (24) ($\hat{A} = \hat{F}^{(\pm)}$), one obtains the matrix representation of the on-shell Fredholm integral (inverse wave) operator as follows [26]:

$$F^{(\pm)}_{\text{on shell}} = (W^{(\pm)}_{\text{on shell}})^{-1} = \begin{bmatrix} 1 & 0 & \pm iu_0 & \pm iu_0 \\ 0 & 1 & \pm iu_0 & \pm iu_0 \\ \pm iu_1 & \pm iu_1 & 1 & 0 \\ \pm iu_1 & \pm iu_1 & 0 & 1 \end{bmatrix}, \tag{77}$$

where the basis functions in the row and column are in the order of $|k_0 0\rangle$, $|-k_0 0\rangle$, $|k_1 1\rangle$, and $|-k_1 1\rangle$, and its determinant is obtained by straightforward calculations:

$$\det \hat{F}^{(\pm)}_{\text{on shell}} = \det(\hat{W}^{(\pm)}_{\text{on shell}})^{-1} = 1 + 4u_0u_1. \tag{78}$$

Then, the on-shell S-matrix element is evaluated by Eq. (34), i.e.,

$$\langle k_{\zeta'}\zeta'|\hat{S}_{\text{on shell}}|k_\zeta\zeta\rangle = \frac{\det(\hat{F}^{(+)}_{\text{on shell}})_{[(k_\zeta\zeta)\bullet \to \langle k_{\zeta'}\zeta'|\hat{F}^{(-)}_{\text{on shell}}|\bullet\rangle]}}{\det \hat{F}^{(+)}_{\text{on shell}}}. \tag{79}$$

As a result, one can construct the following representation of the on-shell S matrix:

$$S_{\text{on shell}} = \frac{1}{1 + 4u_0u_1}\begin{bmatrix} 1 & -4u_0u_1 & -2iu_0 & -2iu_0 \\ -4u_0u_1 & 1 & -2iu_0 & -2iu_0 \\ -2iu_1 & -2iu_1 & 1 & -4u_0u_1 \\ -2iu_1 & -2iu_1 & -4u_0u_1 & 1 \end{bmatrix}. \tag{80}$$

Equation (80) coincides with the far-field amplitude calculated analytically in Appendix B 2. Furthermore, one may check current conservation law (C7) (see Appendix C 2) by a straightforward calculation:

$$(S_{\text{on shell}})^{\dagger}\text{diag}(k_0,k_0,k_1,k_1)S_{\text{on shell}} = \text{diag}(k_0,k_0,k_1,k_1), \tag{81}$$

where diag(…) is a diagonal matrix, of which the diagonal elements are its arguments. The above analytical calculations ensure that our formula for the on-shell S-matrix element is applicable to multichannel inelastic systems.

V. LE COUTEUR–NEWTON FORMULA AS A SPECIAL CASE

In this section, we apply Eq. (34) to the radial part of a three-dimensional multichannel scattering system composed of two particles and show that the Le Couteur–Newton formula [2,3] can be derived as a special case. Suppose a quantum scattering system with a target and traveling particle under the total Hamiltonian $\hat{H}^{(0)}+\hat{V}$, where $\hat{H}^{(0)}$ and $\hat{V}$ are a null-interaction Hamiltonian and the interaction potential operator, respectively. In the subspace specified by the total energy E and total angular momentum (J,M_J), we assume that the total wave function of a scattering state is expressed in the spherical coordinates as

$$\langle r\sigma|\Psi(\pm)\rangle_{\text{radial+internal}} = \sum_i Z_i(\sigma)\frac{1}{r}\langle r|k_i(\pm)\rangle, \tag{82}$$

where r is the radial coordinate of the traveling particle and σ is a set of the internal coordinates, that is, all the coordinates other than r. The channel index i is specified by the internal state $Z_i(\sigma)$, which is an eigenstate of $\hat{H}^{(0)}$ with the internal energy ϵ_i and the total angular momentum (J,M_J). Actually, $Z_i(\sigma)$ is synthesized to have (J,M_J) from the angular part of the traveling-particle state with an orbital angular momentum l_i and the rest part of angular momentums (the spin part of the traveling-particle state and a target state with ϵ_i). $\langle r|k_i(+)\rangle$ is the radial wave function with the incident incoming wave number $k_i=(E-\epsilon_i)^{1/2}$ (real and positive); the suffix for the contraction of the radial part is omitted for simplicity. The contraction of the total Schrödinger equation with the ith internal state, $\langle Z_i|\hat{H}^{(0)}+\hat{V}-E|\Psi\rangle_{\text{internal}}=0$, leads to coupled radial Schrödinger equations [27] in the subspace specified by E and (J,M_J):

$$\left(-\frac{d^2}{dr^2}+\frac{l_i(l_i+1)}{r^2}-k_i^2\right)\langle r|k_i(\pm)\rangle = -\sum_{i'}\int_0^{\infty} dr' V_{ii'}(r,r')\langle r'|k_{i'}(\pm)\rangle,$$

$$i=0,1,2,\ldots. \tag{83}$$

Although the domain is semi-infinite $(0\le r<\infty)$ and the internal states are eliminated by contraction, this is essentially a one-dimensional multichannel inelastic scattering system, which is similar to the system treated in Sec. IV D. Indeed, we may find the retarded and advanced Green's functions in Ref. [28], define Fredholm operator by Eq. (3), and apply Eq. (34) to the calculation of the on-shell S matrix, which determines the asymptotic wave function [see Eqs. (C2) and (C5)] [27]. Then, Eq. (34) reads

$$\langle k_{i'}|\hat{S}_{\text{on shell}}|k_i\rangle = \frac{\det(\hat{W}^{(+)}_{\text{on shell}})^{-1}_{[k_i\bullet\to\langle k_{i'}|(\hat{W}^{(-)}_{\text{on shell}})^{-1}|\bullet\rangle]}}{\det(\hat{W}^{(+)}_{\text{on shell}})^{-1}}$$

$$= \frac{\det(\hat{F}^{(+)}_{\text{on shell}})_{[k_i\bullet\to\langle k_{i'}|\hat{F}^{(-)}_{\text{on shell}}|\bullet\rangle]}}{\det\hat{F}^{(+)}_{\text{on shell}}} \tag{84}$$

$$= \frac{\det(\hat{W}^{(+)}_{\text{on shell}})^{-1}_{[k_i\bullet\to\langle -k_{i'}|(\hat{W}^{(+)}_{\text{on shell}})^{-1}|\bullet\rangle]}}{\det(\hat{W}^{(+)}_{\text{on shell}})^{-1}}$$

$$= \frac{\det(\hat{F}^{(+)}_{\text{on shell}})_{[k_i\bullet\to\langle -k_{i'}|\hat{F}^{(+)}_{\text{on shell}}|\bullet\rangle]}}{\det\hat{F}^{(+)}_{\text{on shell}}} \tag{85}$$

$$= \frac{f(+k_0,\ldots,-k_{i'},\ldots,+k_{i'},\ldots,+k_N)}{f(+k_0,\ldots,+k_i,\ldots,+k_{i'},\ldots,+k_N)}, \tag{86}$$

where f is the Fredholm determinant as a function of the wave numbers that label the row vectors [29]. The argument $-k_{i'}$ in Eqs. (85) and (86) is the natural extension to a negative-valued argument. From Eq. (84) to Eq. (85), we use the following equation derived from Eq. (29) and lemma (C1) proved in Appendix C 1 under an adequate definition for phase of the wave function $\langle r|k_i(\pm)\rangle=\langle r|\hat{W}^{(\pm)}|k_i\rangle$:

$$\langle k_{i'}|(\hat{W}^{(-)}_{\text{on shell}})^{-1} = \langle k_{i'}|(\hat{W}^{(-)^{\dagger}})_{\text{on shell}}$$

$$= \langle -k_{i'}|(\hat{W}^{(+)^{\dagger}})_{\text{on shell}} = \langle -k_{i'}|(\hat{W}^{(+)}_{\text{on shell}})^{-1}. \tag{87}$$

Equation (84) or Eq. (86) is sufficient for practical calculations of both the diagonal and nondiagonal elements of $\hat{S}_{\text{on shell}}$. Now, we demonstrate that our formula (86) leads to the Le Couteur–Newton formula.

The Le Couteur–Newton formula for a diagonal element is the same as Eq. (86). To derive a nondiagonal element, we need lemma (C12) derived in Appendix C 3 and the current conservation law expressed as Eq. (C11) in Appendix C 2. Let us calculate the next quantity using Eq. (86) and lemma (C12) with $C=\hat{F}^{(+)}$:

$$\frac{\det(\hat{F}^{(+)}_{\text{on shell}})_{[k_i\bullet\to\langle k_i|\hat{F}^{(-)}_{\text{on shell}}|\bullet\rangle,k_{i'}\bullet\to\langle k_{i'}|\hat{F}^{(-)}_{\text{on shell}}|\bullet\rangle]}}{\det\hat{F}^{(+)}_{\text{on shell}}}$$

$$= \frac{f(+k_0,\ldots,-k_i,\ldots,-k_{i'},\ldots,+k_N)}{f(+k_0,\ldots,+k_i,\ldots,+k_{i'},\ldots,+k_N)}$$

$$= \langle k_i|\hat{S}_{\text{on shell}}|k_i\rangle\langle k_{i'}|\hat{S}_{\text{on shell}}|k_{i'}\rangle - \langle k_{i'}|\hat{S}_{\text{on shell}}|k_i\rangle\langle k_i|\hat{S}_{\text{on shell}}|k_{i'}\rangle. \tag{88}$$

Equation (88) with the current conservation law (C11) results in the Le Couteur–Newton formula for nondiagonal element. Altogether our formula (34) leads to the Le Couteur–Newton formula, i.e., the next expressions for the diagonal and nondiagonal elements of $\hat{S}_{\text{on shell}}$ in terms of the single function f:

$$\langle k_i|\hat{S}_{\text{on shell}}|k_i\rangle = \frac{f(+k_0,\ldots,-k_i,\ldots,+k_N)}{f(+k_0,\ldots,+k_i,\ldots,+k_N)}, \tag{89}$$

$$\langle k_{i'}|\hat{S}_{\text{on shell}}|k_i\rangle = \frac{k_i}{k_{i'}}\langle k_i|\hat{S}_{\text{on shell}}|k_{i'}\rangle = \left[\frac{k_i}{k_{i'}}\left\{\langle k_i|\hat{S}_{\text{on shell}}|k_i\rangle\langle k_{i'}|\hat{S}_{\text{on shell}}|k_{i'}\rangle - \frac{f(+k_0,\ldots,-k_i,\ldots,-k_{i'},\ldots,+k_N)}{f(+k_0,\ldots,+k_i,\ldots,+k_{i'},\ldots,+k_N)}\right\}\right]^{1/2} \text{for } i' \neq i. \tag{90}$$

Note that there is an ambiguity in the sign for the nondiagonal elements arising from the double-valued property of the square root, although this ambiguity is of no consequence for evaluating the transition probability, which is essentially the intensity of a nondiagonal on-shell S-matrix element.

The Le Couteur–Newton formula is valid in the open-channel space because its derivation relies on the current conservation law (C11). Our formula (34) is also valid in the open-channel space; however, Eq. (34) covers the Le Couteur–Newton formula and possesses extended applicability as shown in Secs. IV C and IV D.

VI. SUMMARY

In conclusion, we have demonstrated the following:

(1) We have developed a general determinantal formulation for direct evaluation of various quantities including local field amplitudes and transition amplitudes (S-matrix elements and T-matrix elements). This formulation is based on the principle that a desired quantity can be extracted from a wave operator that maintains all of the information concerning the system. All the formulas were simply derived using the Fredholm determinant and Cramer's rule.

(2) The formula for the local field amplitude is effective both in the near- and far-field regions. Numerical calculations were demonstrated successfully for one- and three-dimensional elastic (potential) scattering systems.

(3) Our formula for S-matrix elements is effective in the space of open channels. Analytical calculations were demonstrated in simplified multichannel elastic and inelastic scattering systems.

(4) Our formula for S-matrix elements covers the Le Couteur–Newton formula.

The following are remaining problems: (1) direct evaluation of S-matrix elements related to closed channels, (2) application of our formulation to near-field amplitude in an inelastic scattering system, (3) development of a numerical method to evaluate matrix element of on-shell Fredholm integral operator, (4) treatment of a system with vector potential, (5) treatment of a system with rearrangement, and (6) treatment of quantum many-body problems.

At present, our formula needs a relatively larger amount of numerical calculation compared with other methods required to construct the solution. However, the present direct method will be helpful in the analysis and design of near-field-related systems as described in Sec. I.

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APPENDIX A: A SINGULARITY OF THE WAVE OPERATOR ON AN ENERGY SHELL

Here we prove Eq. (19). In a quantum system, Eq. (1) is equivalent to the following Schrödinger equations:

$$\hat{H}^{(0)}|k\rangle = |k\rangle E_k, \tag{A1}$$

$$(\hat{H}^{(0)} + \hat{V})|k(+)\rangle = |k(+)\rangle E_k, \tag{A2}$$

where $\hat{H}^{(0)}$ is a Hamiltonian without a scattering potential and satisfies the following equation on the E_k shell [18]:

$$(E_k \pm i0 - \hat{H}^{(0)})\hat{G}^{(0\pm)} = \hat{1}. \tag{A3}$$

Using Eqs. (1) and (A3), Eq. (19) is proved as follows:

$$\begin{aligned}\langle k'|\hat{W}^{(\pm)}|k\rangle &= \langle k'|k(+)\rangle = \langle k'|k\rangle + \langle k'|\frac{1}{E_k \pm i0 - \hat{H}^{(0)}}\hat{V}|k(+)\rangle \\ &= \langle k'|k\rangle + \frac{1}{E_k - E_{k'} \pm i0}\langle k'|\hat{V}\hat{W}^{(\pm)}|k\rangle \\ &= \langle k'|k\rangle + \left[\mp \pi i\delta(E_k - E_{k'}) + \mathrm{P}\frac{1}{E_k - E_{k'}}\right] \\ &\quad \times \langle k'|\hat{T}^{(\pm)}|k\rangle,\end{aligned} \tag{A4}$$

where $|k'\rangle$ possibly has an off-shell energy $E_{k'}(\neq E_k)$, and we use $1/(x \pm i0) = \mathrm{P}(1/x) \mp \pi i\delta(x)$. The retarded and advanced T-matrix elements have finite values, and thus the matrix element of the wave operator on an energy shell has the same type of singularity as the S operator.

APPENDIX B: ANALYTICAL SOLUTIONS OF PROBLEMS IN Sec. IV

In Appendixes B 1 and B 2, analytical expressions for the far-field amplitude are given to compare with the on-shell S-matrix elements evaluated in Secs. IV C and IV D, respectively.

1. Far-field amplitude in the elastic scattering problem of Sec. IV C

The on-shell S-matrix element represents the transition amplitude and far-field amplitude simultaneously. The wave function $|k_\iota(+)\rangle$ obtained by the incident field $|k_\iota\rangle$ ($k_\iota=+k$ for $\iota=+$ and $k_\iota=-k$ for $\iota=-$) satisfies the next Lippmann-Schwinger equation in abstract vector space:

$$|k_\iota(+)\rangle = |k_\iota\rangle + \hat{G}^{(0+)}\hat{V}|k_\iota(+)\rangle. \tag{B1}$$

The asymptotic wave function on the energy shell can be expanded by the two basis functions as

$$|k_\iota(+)\rangle = c_{+\iota}|k\rangle + c_{-\iota}|-k\rangle, \tag{B2}$$

where $c_{\pm\iota}$ is the coefficient to be determined. The next relationship holds in a one-dimensional elastic scattering system:

$$c_{\iota'\iota} = \langle k_{\iota'}|\hat{S}_{\text{on shell}}|k_\iota\rangle. \tag{B3}$$

To prove Eq. (B3), we calculate the field amplitude using Eqs. (1), (7), (18), (40), and (42):

$$\langle x|k_\iota(+)\rangle = \langle x|\hat{W}^{(+)}|k_\iota\rangle = \langle x|k_\iota\rangle + \int_{-\infty}^{+\infty} dx' \int_{-\infty}^{+\infty} dk' \times \langle x|\hat{G}^{(0+)}|x'\rangle\langle x'|k'\rangle\langle k'|\hat{T}^{(+)}|k_\iota\rangle. \tag{B4}$$

Then, the asymptotic form (far-field amplitude) becomes

$$\sqrt{2\pi}\langle x|k_\iota(+)\rangle \to \exp(ik_\iota x) + \exp(ik|x|)\frac{-2\pi i}{2k}\langle k_o|\hat{T}^{(+)}|k_\iota\rangle \quad \text{as } |x|\to\infty. \tag{B5}$$

For the derivation, we use $|x-x'|\to|x|-x'\frac{x}{|x|}$ as $|x|\to\infty$ and $k_o \equiv k\frac{x}{|x|}$. To find c_{-+}, for example, we set $\iota=+$ and $x\to-\infty$, and compare with Eq. (B2). Then, one obtains $c_{-+}=-2\pi i/(2k)\langle -k|\hat{T}^{(+)}|k\rangle=\langle -k|\hat{S}_{\text{on shell}}|k\rangle$ [see Eq. (25) regarding $\delta(\Omega_{k'}-\Omega_k)$ as $\delta_{k'k}$]. In this way, Eq. (B3) is proved.

Using Eq. (B3), we can check the result in Sec. IV C. We can analytically evaluate $c_{\iota'\iota}$ by solving Eq. (B1). Substituting asymptotic wave function (B2) into Eq. (B1), we obtain

$$c_{+\iota}e^{ikx} + c_{-\iota}e^{-ikx} = e^{ik_\iota x} - 2iue^{ik|x|}(c_{+\iota}+c_{-\iota}), \tag{B6}$$

where u is given in Eq. (59). Now, suppose that the incident field is $|k\rangle$, i.e., $\iota=+$. In the region $x>0$, $c_{-+}=0$ and c_{++} can be determined by comparing both sides of Eq. (B6):

$$c_{++} = \frac{1}{1+2iu}. \tag{B7}$$

In the region $x<0$, $c_{++}=1$, and we obtain

$$c_{-+} = \frac{-2iu}{1+2iu}. \tag{B8}$$

Equations (B7) and (B8) together with Eq. (63) satisfy Eq. (B3). For the incident field with $\iota=-$, the same procedure justifies Eq. (B3). Therefore, the expression for on-shell S matrix (63) obtained by the determinantal method is correct.

2. Far-field amplitude in the inelastic scattering problem of Sec. IV D

Let us treat the system of Sec. IV D tracing the manner of Appendix B 1. The wave function $|k_\iota\iota(+)\rangle$ obtained by the incident field $|k_\iota\iota\rangle \in \{|\pm k_\zeta\zeta\rangle \,|\, \zeta=0,1\}$ satisfies the next Lippmann-Schwinger equation:

$$|k_\iota\iota(+)\rangle = |k_\iota\iota\rangle + \hat{G}^{(0+)}\hat{V}|k_\iota\iota(+)\rangle. \tag{B9}$$

The asymptotic wave function can be expanded using channel functions on the energy shell as

$$|k_\iota\iota(+)\rangle = c_{0\iota}|k_0 0\rangle + c_{\bar{0}\iota}|-k_0 0\rangle + c_{1\iota}|k_1 1\rangle + c_{\bar{1}\iota}|-k_1 1\rangle, \tag{B10}$$

where $c_{\zeta\iota}$ and $c_{\bar{\zeta}\iota}$ are the coefficients to be determined; and ζ and $\bar{\zeta}$ in the suffix of c indicate abbreviation of (k_ζ,ζ) and $(-k_\zeta,\zeta)$, respectively.

In a similar manner as in Appendix B 1, we can prove the next relationship:

$$c_{\iota'\iota} = \langle k_{\iota'}\iota'|\hat{S}_{\text{on shell}}|k_\iota\iota\rangle. \tag{B11}$$

Using Eq. (B11), we can check the result in Sec. IV D. We can analytically evaluate $c_{\iota'\iota}$ by solving Eq. (B9). Substituting Eq. (B10) into Eq. (B9), we obtain

$$\begin{aligned} &c_{0\iota}e^{ik_0x}Z_0(\sigma) + c_{\bar{0}\iota}e^{-ik_0x}Z_0(\sigma) + c_{1\iota}e^{ik_1x}Z_1(\sigma) + c_{\bar{1}\iota}e^{-ik_1x}Z_1(\sigma) \\ &= e^{ik_\iota x}Z_\iota(\sigma) - 2iu_0e^{ik_0|x|}Z_0(\sigma)(c_{1\iota}+c_{\bar{1}\iota}) \\ &\quad - 2iu_1e^{ik_1|x|}Z_1(\sigma)(c_{0\iota}+c_{\bar{0}\iota}), \end{aligned} \tag{B12}$$

where u_ζs are given in Eq. (76). Suppose that the incident field is $|k_0 0\rangle$, i.e., $\iota=0$. In the region $x>0$, $c_{\bar{0}0}=c_{\bar{1}0}=0$, and c_{00} and c_{10} can be determined by comparing both sides of Eq. (B12):

$$c_{00} = \frac{1}{1+4u_0u_1}, \tag{B13}$$

$$c_{10} = \frac{-2iu_1}{1+4u_0u_1}. \tag{B14}$$

In the region $x<0$, $c_{00}=1$, $c_{10}=0$, and we obtain

$$c_{\bar{0}0} = \frac{-4u_0u_1}{1+4u_0u_1}, \tag{B15}$$

$$c_{\bar{1}0} = \frac{-2iu_1}{1+4u_0u_1}. \tag{B16}$$

Equations (B13)–(B16) together with Eq. (80) satisfy Eq. (B11). In the other cases with the incident field labeled by

$\iota=\bar{0},1,\bar{1}$, the same procedure justifies Eq. (B11). Therefore, the expression for on-shell S matrix (80) obtained by the determinantal method is correct.

APPENDIX C: LEMMAS FOR Sec. V

Here, we give the lemmas and the current conservation law that are required for the proof in Sec. V.

1. Lemma for Eq. (87)

To make Eq. (87) complete, we prove the next lemma:

$$\langle k_i|(\hat{W}^{(-)\dagger})_{\text{on shell}} = \langle -k_i|(\hat{W}^{(+)\dagger})_{\text{on shell}}, \tag{C1}$$

where k_i is real and positive, and the argument $-k_i$ in the right-hand side is the natural extension to a negative-valued argument. Equation (C1) holds under an adequate definition of the phase in wave functions, $\langle r|\hat{W}^{(\pm)}|k_i\rangle$.

Suppose a general solution of Eq. (83) on the shell with energy E. If the interaction is short range, the asymptotic form at a position of large r is

$$\sum_{n\in E \text{ shell}} \left\{ -A_n \exp\left[+i\left(k_n r - \frac{\pi}{2} l_n\right)\right] + B_n \exp\left[-i\left(k_n r - \frac{\pi}{2} l_n\right)\right]\right\}, \tag{C2}$$

where n runs over all of the open channels on the shell specified by E and (J,M_J). Now let us determine the retarded and advanced solutions as follows: $\langle r|\hat{W}^{(+)}|k_i\rangle$ is the solution satisfying the outgoing boundary condition with an incoming incidence $B_n=+\delta_{ni}\exp(+i\pi l_i/2)$, and $\langle r|\hat{W}^{(-)}|k_i\rangle$ is the solution satisfying the incoming boundary condition with an outgoing incidence $A_n=-\delta_{ni}\exp(-i\pi l_i/2)$. At this point, we have adequately fixed the overall phase through the phase of the incidence, so that a redundant phase factor does not appear in Eq. (C1). Then, the asymptotic form of $\langle r|\hat{W}^{(-)}|k_i\rangle$ on the sphere can be expressed as

$$\begin{aligned}\frac{1}{C_{k_i}}\langle r|\hat{W}^{(-)}|k_i\rangle &= (-1)^{l_i}\exp(+ik_i r) - \sum_{n\in E \text{ shell}} B_n^{(-)} \exp(-ik_n r) \\ &= (-1)^{l_i}\exp[-i(-k_i)r] \\ &\quad - \sum_{n\in E \text{ shell}} A_n^{(+)} \exp[+i(-k_n)r] \\ &= \frac{1}{C_{k_i}}\langle r|\hat{W}^{(+)}|-k_i\rangle,\end{aligned} \tag{C3}$$

where C_{k_i} is the real normalization factor determined from Eq. (10); $B_n^{(-)}$ and $A_n^{(+)}(=B_n^{(-)})$ are introduced to distinguish the two possible interpretations for the same state; and the last expression holds if one permits a negative value of the channel wave number. A solution to the radial Schrödinger equation is uniquely determined by the boundary condition at r, so that the next relation holds:

$$\hat{W}^{(-)}|k_i\rangle = \hat{W}^{(+)}|-k_i\rangle. \tag{C4}$$

The Hermite conjugate of Eq. (C4) and the definition of on-shell wave operator, Eq. (24) ($\hat{A}=\hat{W}^{(\pm)\dagger}$), lead to lemma (C1) under the definition that $E_{-k_i}=E_{k_i}$.

2. Current conservation law in terms of the S matrix

Following Ref. [2], we derive the current conservation law applicable to inelastic scattering systems, which is expressed by the radial Schrödinger equation (83) in the *semi-infinite* domain. The on-shell S matrix determines asymptotic field amplitude (C2) as [27]

$$A_{i'} = \sum_{i\in E \text{ shell}} \langle k_{i'}|\hat{S}_{\text{on shell}}|k_i\rangle B_i. \tag{C5}$$

Current conservation for open channels (with real wave numbers) is expressed as

$$\sum_{i\in E \text{ shell}} \sum_{i'\in E \text{ shell}} A_{i'}^* \delta_{i'i} k_i A_i = \sum_{i\in E \text{ shell}} \sum_{i'\in E \text{ shell}} B_{i'}^* \delta_{i'i} k_i B_i, \tag{C6}$$

where the diagonal matrix $\delta_{i'i}k_i$ is the wave number representation of the operator for the absolute value of momentum along the radial direction. Eliminating A_is in Eq. (C6) using Eq. (C5), one obtains

$$\sum_{j\in E \text{ shell}} \sum_{j'\in E \text{ shell}} \langle k_{i'}|(\hat{S}_{\text{on shell}})^\dagger|k_{j'}\rangle \delta_{j'j} k_j \langle k_j|\hat{S}_{\text{on shell}}|k_i\rangle = \delta_{i'i}k_i. \tag{C7}$$

Equation (C7) corresponds to the unitarity of the on-shell S matrix in an inelastic multichannel system. Although we have here examined the system treated in Sec. V, Eq. (C7) is effective for a general system.

Let us derive another form of Eq. (C7) specific to the system expressed by radial Schrödinger equation (83). The time reversal of Eq. (C2) becomes

$$\sum_{n\in E \text{ shell}} \left\{ -A_n^* \exp\left[-i\left(k_n r - \frac{\pi}{2} l_n\right)\right] + B_n^* \exp\left[+i\left(k_n r - \frac{\pi}{2} l_n\right)\right]\right\}, \tag{C8}$$

where * indicates the complex conjugate. Equation (C8) is also the general solution in the same domain subspace and should be equivalent to Eq. (C2). That is, the on-shell S matrix satisfies

$$B_{i'}^* = \sum_{i\in E \text{ shell}} \langle k_{i'}|\hat{S}_{\text{on shell}}|k_i\rangle A_i^*. \tag{C9}$$

Equations (C5) and (C9) lead to

$$\langle k_{i'}|\hat{S}_{\text{on shell}}|k_i\rangle^* [= \langle k_i|(\hat{S}_{\text{on shell}})^\dagger|k_{i'}\rangle] = \langle k_{i'}|(\hat{S}_{\text{on shell}})^{-1}|k_i\rangle. \tag{C10}$$

Finally, Eqs. (C7) and (C10) result in

$$k_{i'}\langle k_{i'}|\hat{S}_{\text{on shell}}|k_i\rangle = k_i\langle k_i|\hat{S}_{\text{on shell}}|k_{i'}\rangle. \tag{C11}$$

The Le Couteur–Newton formula derived in [2,3] essentially relies on Eq. (C11) and is therefore applicable in the domain with open channels.

Note that relationship (C11) is not applicable to the system with an *infinite* domain as treated in Secs. IV C and IV D. We should consider the asymptotic wave function in the limits of $x\to+\infty$ and $x\to-\infty$ simultaneously, and the relationship corresponding to Eq. (C11) is somewhat complicated.

3. Lemma for Eq. (88)

Let us prove the following lemma:

$$\det C_{[a\bullet\to A_\bullet]}\det C_{[b\bullet\to B_\bullet]} - \det C_{[a\bullet\to B_\bullet]}\det C_{[b\bullet\to A_\bullet]} = \det C_{[a\bullet\to A_\bullet, b\bullet\to B_\bullet]}\det C. \tag{C12}$$

The proof proceeds as follows:

$$[\text{the left-hand side of (C12)}] \tag{C13}$$

$$= \sum_{i,j,i',j'}\left\{\begin{vmatrix} A_i & A_j \\ C_{bi} & C_{bj}\end{vmatrix}\cdot\begin{vmatrix} C_{ai'} & C_{aj'} \\ B_{i'} & B_{j'}\end{vmatrix} - \begin{vmatrix} B_i & B_j \\ C_{bi} & C_{bj}\end{vmatrix}\cdot\begin{vmatrix} C_{ai'} & C_{aj'} \\ A_{i'} & A_{j'}\end{vmatrix}\right\}\tilde{C}_{(ab)(ij)}\tilde{C}_{(ab)(i'j')} \tag{C14}$$

$$= \sum_{i,j,i',j'}\left\{\begin{vmatrix} A_i & A_j \\ B_i & B_j\end{vmatrix}\cdot\begin{vmatrix} C_{ai'} & C_{aj'} \\ C_{bi'} & C_{bj'}\end{vmatrix}\right\}\tilde{C}_{(ab)(ij)}\tilde{C}_{(ab)(i'j')} \tag{C15}$$

$$= [\text{the right-hand side of (C12)}], \tag{C16}$$

where $\tilde{C}_{(ab)(ij)}$ is a cofactor; and (ab) and (ij) are two rows and two columns to be eliminated from the original matrix C, respectively. From Eq. (C13) to Eq. (C14) and from Eq. (C15) to Eq. (C16), we employ the Laplace expansion theorem [22], e.g.,

$$\det C = \sum_{i,j}\begin{vmatrix} C_{ai} & C_{aj} \\ C_{bi} & C_{bj}\end{vmatrix}\tilde{C}_{(ab)(ij)} \quad \text{for} \quad \forall\ a\neq b. \tag{C17}$$

One can check the equality of Eqs. (C14) and (C15) by an explicit calculation of the determinants of the 2×2 matrices in $\{\}$. The next replacements in lemma (C12) lead to Eq. (88): $C\to\hat{F}^{(+)}_{\text{on shell}}$, $A_\bullet\to\langle k_i|\hat{F}^{(-)}_{\text{on shell}}|\bullet\rangle$ and $B_\bullet\to\langle k_{i'}|\hat{F}^{(-)}_{\text{on shell}}|\bullet\rangle$.

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[20] Reference [4], Sec. 6.4.
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[25] The two degrees of freedom of the channels essentially come from parity (inner degrees of freedom). Although $|k\rangle$ and $|-k\rangle$ as the initial and/or final states do not possess well-defined parity, the equivalent basis $|k,\text{even}\rangle \equiv (|k\rangle + |-k\rangle)/\sqrt{2}$ and $|k,\text{odd}\rangle \equiv (|k\rangle - |-k\rangle)/(\sqrt{2}i)$ possess even and odd parities, respectively. We may decompose the problem into two single-channel problems specified by parity; however, we would like to treat a multichannel problem here to keep the applicability to systems without spatial inversion symmetry.

[26] Here we demonstrate the calculation in a similar manner as in Sec. IV C. One can more easily obtain the result using relationship (A3).

[27] Reference [4], Sec. 16.4 (for our case, ignore the labels for arrangement channel in this reference).

[28] Reference [4], Sec. 11.1.

[29] In ordinary notation of the scattering problem with a semi-infinite domain of the radial part, the initial channel function with the label k_i and the final one with the same label represent different functions. The former appears in "ket" of the S-matrix element and $\langle r|k_i\rangle \sim \exp(-ik_i r)$ (incoming field), while the latter appears in "bra" and $\langle k_i|r\rangle^* \sim [\exp(ik_i r)]^*$ (outgoing field). This situation is different from the models in Sec. IV, where the label possesses a common meaning for the initial and final channels. However, it is merely a convention that the labels in "bra" and "ket" carry different meanings, and it is of no consequence to the definition of the S matrix.