Optical Potentials for Inelastic Scattering from Many-Body Targets

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The standard text book Green's function possesses a self-energy that is known to be an optical potential for *elastic* scattering. The introduction of an optical potential reduces the complex many-body scattering problem into a tractable one-body problem. In this paper inelastic Green's functions are introduced and discussed which possess self-energies that are optical potentials for *inelastic* scattering. If the projectile is indistinguishable from particles comprising the target, intriguing aspects arise even for noninteracting particles.

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To investigate *elastic* scattering of a projectile from a many-body target in its ground state $|0\rangle$, common text books introduce a quantity called one-particle Green's function (GF) [1–4]

$$\begin{aligned} g_{pq}(t,t') &= g^{+}_{pq} + g^{-}_{pq} \\ &\equiv -i\theta(t-t')\langle 0|b_p(t)b^{\dagger}_q(t')|0\rangle \\ &\quad + i\theta(t'-t)\langle 0|b^{\dagger}_q(t')b_p(t)|0\rangle, \end{aligned} \tag{1}$$

where b_p and $b^{\dagger}_p$ denote annihilation and creation operators for projectiles in projectile one-particle states φ_p. This GF is subject to the well-known Dyson equation, which, after Fourier transformation from time to energy space, reads in matrix notation [1–4]

$$\boldsymbol{g}(\omega) = \boldsymbol{g}^{(0)}(\omega) + \boldsymbol{g}^{(0)}(\omega)\boldsymbol{\sigma}(\omega)\boldsymbol{g}(\omega). \tag{2}$$

Here $\boldsymbol{g}^0$ denotes the free GF computed without particle-particle interaction. Equation (2) connects the GF with its kernel $\boldsymbol{\sigma}(\omega)$, which is called self-energy. Among the many interesting properties of the self-energy is that it represents an effective energy-dependent *one-particle* potential which is an exact optical potential for elastic scattering [5]; i.e., scattering calculations performed with the one-particle potential $\boldsymbol{\sigma}(\omega)$ provide exact elastic scattering data on the many-body system under investigation.

The construction of optical potentials for elastic scattering and their application has been a vivid field of research in several areas (see, e.g., Refs. [6–9]). Inelastic processes play a central role in nature and there are ample experimental data on various inelastic cross sections. Although the usefulness of an available optical potential for computing inelastic scattering is self-evident, the problem of constructing one or even proving its existence has resisted solution. It is the goal of this paper to investigate possible solutions to the problem.

Before turning to the optical potential for inelastic scattering it is illuminating to briefly investigate the standard GF (1). By remembering the Heisenberg representation for operators, $b(t) = e^{iHt}be^{-iHt}$, the GF is readily interpreted. For convenience we choose the ground state energy of the target as the origin of the energy scale and put $\tau = t - t'$. At time zero a particle is attached to the ground state of the target. This compound state propagates as usual via the total Hamiltonian H of the system: $e^{-iH\tau}b^{\dagger}_q|0\rangle$. At time $\tau > 0$ we ask for the probability of finding $b^{\dagger}_p|0\rangle$ in this compound state. Apart from a trivial prefactor $-i$, this autocorrelation function is exactly the advanced-particle [10] GF, $\boldsymbol{g}^+$, in Eq. (1). From this interpretation it is clear that $\boldsymbol{g}^+$ describes elastic scattering. However, $\boldsymbol{g}^+$ is not invertible and cannot be used to construct a well-behaved optical potential [6,11]. To remedy the situation the retarded-hole GF, $\boldsymbol{g}^-$, is needed. This quantity is the autocorrelation function of a hole state $e^{+iH\tau}b_p|0\rangle$ which can be interpreted as a particle going backward in time [1]. $\boldsymbol{g}^-$ is also not invertible, but $\boldsymbol{g} = \boldsymbol{g}^+ + \boldsymbol{g}^-$ is invertible because of the anticommutator relation $b_pb^{\dagger}_q + b^{\dagger}_qb_p = \delta_{pq}$ for fermions. By using a slight redefinition of $\boldsymbol{g}$, analogous results are obtained for bosons [1].

Let us briefly compare different projectile particles. If the projectile is distinguishable from the particles composing the target, a situation encountered in, e.g., the scattering of a positron from atoms and molecules, the GF simplifies [12]. The retarded-hole GF vanishes since one cannot annihilate a positron in the target. On the other hand, if the projectile is indistinguishable from particles comprising the target, both the retarded-hole and advanced-particle GFs are needed to accommodate the fermion anticommutator relation and determine a well-behaved, i.e., nonsingular, optical potential. The presence of both a particle state and a hole state appropriately propagating in time reflects the particle-hole symmetry inherent in the GF and hence also in the optical potential of indistinguishable particles.

The above discussion in terms of propagating particle and hole states or, equivalently, multiparticle wave packets straightforwardly leads to the definition of GFs for inelastic processes. At time zero a particle is attached to an arbitrary state $|M\rangle$ of the target and this wave packet propagates in time as $e^{-iH\tau}b^{\dagger}_q|M\rangle$. A set of advanced-particle GFs is obtained by asking for the probabilities of finding $b^{\dagger}_p|N\rangle$ in the wave packet, i.e., by computing cross-correlation functions. Analogously, the cross-correlation functions of the hole states $e^{+iH\tau}b_p|M\rangle$ determine the retarded-hole

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GFs. The results read

$$G_{pq}^{[N,M]}(t,t') = G_{pq}^{+[N,M]} + G_{pq}^{-[N,M]},$$
$$G_{pq}^{+[N,M]} = -i\theta(t - t')\langle N|b_p(t)b_q^\dagger(t')|M\rangle \times \exp[i\Phi^{+[N,M]}(t,t')],$$
$$G_{pq}^{-[N,M]} = +i\theta(t' - t)\langle N|b_q^\dagger(t')b_p(t)|M\rangle \times \exp[i\Phi^{-[N,M]}(t,t')]. \quad (3)$$

Particular attention should be paid to the phases $\Phi^{\pm}(t,t')$ which are time dependent and different for the advanced-particle and retarded-hole GF:

$$\Phi^{+[N,M]}(t,t') = \Phi^{-[N,M]}(t',t) = -E^{[N]}t + E^{[M]}t'. \quad (4)$$

Note that $\Phi^-(t,t')$ is obtained from $\Phi^+(t,t')$ by interchanging t and t'. $E^{[N]}$ denotes the energy of the target in the state $|N\rangle$.

For obvious reasons we shall call the GF in (1) and (3) the elastic and inelastic GF, respectively. By construction the inelastic GF is time-translational invariant as is the elastic one. Its Fourier transform into energy space reads

$$G_{pq}^{[N,M]}(\omega) = \sum_s \frac{\langle N|b_p|s\rangle\langle s|b_q^\dagger|M\rangle}{\omega - E_{n+1}^{[s]}} + \sum_r \frac{\langle N|b_q^\dagger|r\rangle\langle r|b_p|M\rangle}{\omega + E_{n-1}^{[r]}}, \quad (5)$$

where $|s\rangle$ and $E_{n+1}^{[s]}$ are the eigenstates and energies of the target with one additional particle, and $|r\rangle$ and $E_{n-1}^{[r]}$ are the corresponding quantities of the target with one particle less, i.e., of the ionized target. In principle, all of the inelastic GFs, $\boldsymbol{G}^{[N,M]}$, possess the same poles. By noting that $G_{pq}^{[0,0]} = g_{pq}$, it is obvious that these poles coincide with those of the elastic GF. From a practical point of view this is a very valuable property since no additional poles must be computed for describing inelastic processes.

It is convenient to view $G_{pq}^{[N,M]}$ as matrix elements of a supermatrix $\boldsymbol{G}$ in a double index space, one characterizing the projectile and the other the target. In other words, the pairs (p,N) and (q,M) are the indices of the supermatrix $\boldsymbol{G}$. In complete analogy to (2) this supermatrix fulfills a generalized Dyson equation

$$\boldsymbol{G}(\omega) = \boldsymbol{G}^{(0)}(\omega) + \boldsymbol{G}^{(0)}(\omega)\boldsymbol{\Sigma}(\omega)\boldsymbol{G}(\omega), \quad (6)$$

with a self-energy $\boldsymbol{\Sigma}(\omega)$ as a kernel and a free GF, $\boldsymbol{G}^{(0)}(\omega)$. The target states $|N\rangle$ define the scattering channels. We may define $\boldsymbol{G}(\omega)$ to include as many channels as desired by numbering the channels and setting $N,M \le K$, where K can range from zero to infinity. $K = 0$ implies that only elastic scattering from the target ground state is considered; i.e., $\boldsymbol{G}(\omega)$ comprises only the elastic GF, $\boldsymbol{g}(\omega)$. We stress that the self-energy $\boldsymbol{\Sigma}(\omega)$ of the inelastic GF is an *exact* optical potential for inelastic scattering if the free GF is chosen appropriately [13]. The effect of all inelastic channels $N,M > K$ is absorbed into this exact potential.

One choice of the free GF is that $\boldsymbol{G}^{(0)}(\omega)$ takes on the same appearance as for a projectile distinguishable from the target's particles [12]:

$$G_{pq}^{(0)[N,M]}(\omega) = \frac{\delta_{pq}\delta_{NM}}{(\omega - e_p - E^{[N]})}, \quad (7)$$

where $e_p = \frac{p^2}{2}$ denotes the energy of the projectile with momentum p. Note that the free elastic GF in (2) is given by (7) for $N = M = 0$.

While the free elastic GF, $\boldsymbol{g}^{(0)}(\omega)$, entering the Dyson equation (2) is identical with the computed GF neglecting the interaction between *all* particles, this is surprisingly not the case for the free inelastic GF. Without any interaction $H = H_0 = \sum_k e_k b_k^\dagger b_k$, and the states and energies appearing in (5) become Slater determinants and sums over one-particle energies e_k. It is rather straightforward to show that $G_{pq}^{[N,M]}(\omega)$ coincides with $G_{pq}^{(0)[N,M]}(\omega)$ for $N = M$, but not for $N \ne M$, where the former quantity does not vanish. This nondiagonal structure of the inelastic GF for noninteracting particles has striking consequences: the self-energy $\boldsymbol{\Sigma}(\omega)$ does not vanish, giving rise to a nonvanishing optical potential for inelastic scattering. This potential consists of a static $\boldsymbol{\Sigma}(\infty)$, i.e., energy independent, and a dynamic, i.e., energy dependent, term. The static term has a simple appearance,

$$\Sigma_{pq}^{[N,M]}(\infty) = -\langle N|b_q^\dagger b_p|M\rangle(E^{[N]} + E^{[M]}), \quad (8)$$

and the expression for the dynamic term is more involved and will be given elsewhere [13]. Both terms depend only on target one-particle densities and energies and disappear for the elastic channel $N = M = 0$ (remember that the target ground state has been chosen as the zero of the energy scale).

It is indeed surprising that noninteracting particles do have an obviously nonvanishing scattering potential. Is there a scattering cross section for the scattering of noninteracting particles? The answer is clearly no (see below for proof). Let us consider the scattering of an electron from an atom with n electrons. After the scattering event, one measures an electron and implicitly assumes that it is the scattered projectile. However, one cannot tell which of the $n + 1$ electrons has been measured. The scattering potential is the result of the particles being indistinguishable. In addition, we have shown that one can choose a single channel (here the ground state) for which the elastic optical potential vanishes. Equation (8) implies static coupling between the elastic and inelastic channels. To compensate for this coupling, i.e., to lead to a vanishing elastic optical potential $\boldsymbol{\sigma}$ [see (2)], the inelastic potential must contain dynamical terms in addition to the static terms [(8)].

The inelastic optical potential of the GF in (3) and (4) derived above is not straightforward to evaluate for noninteracting particles and even more so for interacting ones. Can we redefine the GF such that the optical potential vanishes for noninteracting particles and is still an *exact* potential in the general case? The answer is yes. To prove this statement it is helpful to note that optical potentials are not unique quantities, i.e., there are different choices of optical potentials which lead exactly to the same scattering S matrix [6,8]. Consequently, it is a legitimate task to search for another optical potential which gives rise to the same physics, but exhibits the desired appearance. To this end we have to recall that above we have imposed particle-hole symmetry on the inelastic GF in analogy to that inherent in the standard textbook elastic GF. By appropriately breaking this symmetry, we can accomplish our goal. Since the advanced-particle GF, $\boldsymbol{G}^+$, is responsible for the scattering, we have to leave it unchanged [14]. Hence it is $\boldsymbol{G}^-$ which must be redefined. We leave this retarded-hole GF as is and only enforce on it the phase of the advanced-particle one, i.e., we now choose [in Eq. (3)] Φ^- to be identical to Φ^+ [see Eq. (4)]. It should be stressed that this choice of phase maintains the time-translational invariance of the GF. At first sight it might be surprising that a change of phase can have a relevant impact. A closer look reveals, however, that this phase changes substantially the pole structure of $\boldsymbol{G}^-$ in energy space, which now reads

$$G_{pq}^{-[N,M]}(\omega) = \sum_r \frac{\langle N|b_q^\dagger|r\rangle\langle r|b_p|M\rangle}{\omega + E_{n-1}^{[r]} - E^{[N]} - E^{[M]}} . \quad (9)$$

Obviously, the number of poles of $\boldsymbol{G}^-$ has markedly grown and now depends on the channels N and M.

The redefined GF fulfills a generalized Dyson equation (6) with $\boldsymbol{\Sigma}$ again being an exact optical potential for inelastic scattering. The free GF, $\boldsymbol{G}^{(0)}$, is again that given in (7). However, in contrast to the situation elaborated above, this $\boldsymbol{G}^{(0)}$ is now identical with the full GF, $\boldsymbol{G}$, computed for noninteracting particles. In short, the new inelastic optical potential vanishes for noninteracting particles. We pay for violating the particle-hole symmetry by the substantial increase of the number of poles in the retarded-hole GF, which makes practical calculations more cumbersome.

We would like to mention that the redefined, i.e., particle-hole symmetry-broken inelastic GF is amenable to a systematic theoretical evaluation [13]. The resulting inelastic optical potential reads, in matrix notation,

$$\boldsymbol{\Sigma}(\omega) = \boldsymbol{W} + \boldsymbol{V\rho} + \tfrac{1}{4}\boldsymbol{V}^\dagger \boldsymbol{R}(\omega)\boldsymbol{V} . \quad (10)$$

The static term, $\boldsymbol{\Sigma}(\infty) = \boldsymbol{W} + \boldsymbol{V\rho}$, contains the projectile-nuclei interaction $\boldsymbol{W}$ and the electrostatic and exchange interaction $\boldsymbol{V}$ of the projectile with the correlated one-particle densities $\boldsymbol{\rho}$ of the target [see (8)]. The dynamic term is at least of second order in the particle-particle interaction. The inelastic response function $\boldsymbol{R}(\omega)$ depends on the number of channels to be explicitly considered. It fulfills an equation of motion which can be exploited. Details will be given elsewhere [13].

It is concluded that optical potentials for inelastic scattering represent an intricate and intriguing problem when the projectile is indistinguishable from particles comprising the many-body target. Maintaining the particle-hole symmetry inherent in the elastic standard textbook optical potential also in the inelastic potential leads to a nonvanishing potential even for noninteracting particles. The corresponding GF has a particularly simple appearance, but its optical potential is difficult to evaluate. For interacting particles this evaluation is still an open problem. By appropriately violating the particle-hole symmetry, we encounter a GF which gives rise to an inelastic optical potential which vanishes for noninteracting particles and can be evaluated theoretically.

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[1] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, NY, 1971).
[2] E. N. Economou, *Green's Functions in Quantum Physics* (Plenum, NY, 1981).
[3] A. B. Migdal, *Theory of Finite Systems and Applications to Atomic Nuclei* (Wiley, NY, 1971).
[4] G. D. Mahan, *Many-Particle Physics* (Plenum, NY, 1981).
[5] J. S. Bell and E. J. Squires, Phys. Rev. Lett. **3**, 96 (1959).
[6] F. Capuzzi and C. Mahaux, Ann. Phys. (N.Y.) **239**, 57 (1995).
[7] T. N. Rescigno *et al.,* Phys. Rev. Lett. **63**, 248 (1989).
[8] H.-D. Meyer, J. Phys. B **25**, 2657 (1992).
[9] J. Brand *et al.,* Phys. Rev. A **60**, 2983 (1999).
[10] P. Roman, *Advanced Quantum Theory* (Addison-Wesley, Reading, MA, 1965).
[11] J. Brand and L. S. Cederbaum, Ann. Phys. (N.Y.) **252**, 276 (1996).
[12] L. S. Cederbaum, Few-Body Syst. **21**, 211 (1996).
[13] L. S. Cederbaum (to be published).
[14] It is useful to relate the elements of the usual S matrix for inelastic scattering to the inelastic GF. The scattering states of the system with incoming and outgoing boundary conditions can be expressed using creation operators [15]. Since the S matrix is obtained as the scalar product of these states [16], it is straightforward to arrive at the following relation [12]:
$$S(p'N \leftarrow pM) = i \lim_{\substack{t\to+\infty \\ t'\to-\infty}} e^{[E(t-t')]} G_{p'p}^{+[N,M]}(t,t') ,$$
where p is the momentum of the incoming projectile and p' is the momentum after exciting the target from the state $|M\rangle$ to the state $|N\rangle$. E denotes the total energy of the projectile plus target which is a conserved quantity. In the above expression we can augment $\boldsymbol{G}^+$ by any choice of the retarded-hole GF, $\boldsymbol{G}^-(t,t')$, as the latter vanishes for $t > t'$. In other words, we may replace $\boldsymbol{G}^+$ in the above expression by a full GF, $\boldsymbol{G} = \boldsymbol{G}^+ + \boldsymbol{G}^-$, as long as we leave $\boldsymbol{G}^+$ unchanged. We should mention that even if $\boldsymbol{G}$ fulfills a generalized Dyson equation its self-energy $\boldsymbol{\Sigma}$ is not necessarily an optical potential. For $\boldsymbol{\Sigma}$ to be an optical potential it is relevant that $\boldsymbol{G}^0$ itself describes a scattering process [see, e.g., Eq. (7)].
[15] M. Namiki, Prog. Theor. Phys. **23**, 629 (1960).
[16] B. H. Bransden, *Atomic Collision Theory* (Benjamin-Cummings, London, 1983).