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LETTER TO THE EDITOR

Scattering from open-shell many-body targets

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Abstract

The standard one-particle Green function (GF) is extended to account for scattering from open-shell many-body targets. This extended GF possesses a self-energy which is an *exact* optical potential (OP) for scattering from open-shell targets. Furthermore, to *each* scattering process with well-defined quantum numbers there is a *specific* OP, thus reducing the multichannel problem to single-channel ones. As an explicit example we work out, in detail, the scattering of spin-$\frac{1}{2}$ projectiles from open-shell targets.

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Elastic scattering is a basic experimental tool used for studying the internal structure of composite many-body targets. In comparison with closed-shell targets, scattering from open-shell targets is more intricate since for *any* energy of the projectile the scattering process is, in general, a multichannel one. In particular, spin-flips and zero-energy excitations are examples of open channels due to the exchange interaction, even if spin–orbit and spin–spin couplings are negligible. There are ample experimental examples of scattering from open-shell targets, including cases where either the projectiles and/or the targets are polarized, thus enabling one to detect the above-mentioned quantum effects. We mention here the scattering of protons and neutrons from nuclei (^{3}He [1], ^{12}C, ^{28}Si and others [2]) and the scattering of electrons from atoms (Cs, Mn and others [3, 4]), ions (Ar^+ [5]) and molecules (O_2 and NO [4]).

For open-shell atoms and molecules it is possible to successfully compute scattering matrix (*S*-matrix) elements (see, e.g., [6]). For nuclei, where the underlying potentials are not accurately known, and for larger molecules, where the computational effort is substantial, it is a very attractive concept to describe the scattering from the many-body target by an effective one-particle potential (optical potential (OP)). The construction of OPs for elastic scattering from many-body targets and their application has been a vivid field of research in nuclear, atomic and molecular physics (see, e.g., [7, 8] and references therein). Both Feshbach's OPs [9] (constructed by projection operators applied to the coupled-channel equations) and that of Bell and Squires [10] (the self-energy of the one-particle Green function (GF)) are *exact* OPs for elastic scattering from the closed-shell many-body system under investigation. However, for open-shell targets the standard one-particle GF [11] does not apply and, independently, Feshbach's OPs are not well-behaved potentials [7]. It is instructive to mention that, by neglecting the antisymmetrization between the projectile and the target and by adopting the impulse approximation, Kerman *et al* [12] have developed a successful OP for high-energy nucleon–nucleus scattering. To the best of our knowledge, a general OP for elastic scattering from open-shell targets, valid for all projectile's energies, does not appear in the literature. It is the purpose of this letter to construct *exact* OPs for elastic scattering from open-shell many-body targets. It should be emphasized that, although we speak of energetically-elastic scattering, the scattering dynamics is that of a *multichannel* problem, since the target can occupy different states before and after the collision.

Having in mind the construction of a theory that generalizes the text-book GF [11], we mention that for degenerate targets the statistical average of one-particle GFs (defined with respect to each member of the degenerate manifold) has been introduced as an analogue of the usual one-particle GF [13]. Indeed, the statistical GF admits the correct density, particle-number and energy of the degenerate ground state. Moreover, correct energy splittings and relative spectral intensities in ionization of open-shell targets can be extracted from the statistical GF [14]. Unfortunately, its self-energy *is not* an OP for elastic scattering from degenerate targets, owing to its definition as an averaged quantity.

Aiming at constructing OPs for such scattering processes, we therefore resort to another line of reasoning that has been suggested recently by one of the authors [15]. In [15] it has been shown that OPs for inelastic scattering from many-body targets can be formally constructed. The evaluation of these OPs is still an open question, owing to the complexity characterizing the scattering of projectiles indistinguishable from the particles comprising the many-body targets [15]. Below we show that if one restricts the discussion of inelastic scattering to scattering from a degenerate ground state, it is then possible to define a generalized GF (hereafter referred to as the open-shell Green function (OSGF)) which is to scattering from open-shell targets what the standard GF is to scattering from closed-shell targets.

Before defining the OSGF, it is instructive to examine the structure of the standard one-particle GF [11]:

$$\begin{aligned} g_{pq}(t,t') &= g^{+}_{pq}(t,t') + g^{-}_{pq}(t,t') \\ &= -\mathrm{i}\theta(t-t')\langle 0|a_p(t)a^{\dagger}_q(t')|0\rangle + \mathrm{i}\theta(t'-t)\langle 0|a^{\dagger}_q(t')a_p(t)|0\rangle. \end{aligned} \tag{1}$$

Here $|0\rangle$ stands for the target's non-degenerate ground state and $a_p(t)$ and $a^{\dagger}_p(t)$ denote the annihilation and creation operators for projectiles in projectile one-particle states φ_p. Throughout this letter we treat fermions exclusively. Adaptation of the formalism and formulae to bosons is straightforward. The advanced-particle GF, $g^{+}_{pq}(t,t')$, represents the scattering process $a^{\dagger}_q|0\rangle \to a^{\dagger}_p|0\rangle$. The retarded-hole partner, $g^{-}_{pq}(t,t')$, is responsible for the complementary process of ionization (electron detachment). $g_{pq}(t,t')$ is subject to the well known Dyson equation, which after Fourier transformation from time-to-energy space, reads in matrix notation [11]

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

$\boldsymbol{g}^{0}(\omega)$ denotes the free GF computed without particle–particle interaction. As mentioned above, the self-energy $\boldsymbol{\sigma}(\omega) = \boldsymbol{\sigma}(\infty) + \boldsymbol{m}(\omega)$ is an *exact* OP for elastic scattering from the system under investigation [10]. $\boldsymbol{\sigma}(\infty)$ and $\boldsymbol{m}(\omega)$ are referred to as the static (energy-independent) and dynamical (energy-dependent) parts of the self-energy.

In scattering from degenerate targets, different channels of the type $a^{\dagger}_q|N\rangle \to a^{\dagger}_p|M\rangle$ are *a priori* possible. $|M\rangle$ and $|N\rangle$ denote two orthogonal states of the ground state manifold. Comparing this to scattering from closed-shell targets suggests the following (intuitive) super-matrix structure for the OSGF:

$$
\begin{aligned}
G_{pq}^{[M,N]}(t,t') &= G_{pq}^{+[M,N]}(t,t') + G_{pq}^{-[M,N]}(t,t') \\
&= -\mathrm{i}\theta(t-t')\langle M|a_p(t)a_q^{\dagger}(t')|N\rangle + \mathrm{i}\theta(t'-t)\langle M|a_q^{\dagger}(t')a_p(t)|N\rangle.
\end{aligned} \tag{3}
$$

M and N are target indices and range over the entire ground state manifold. It is clear that the advanced-particle part, $G_{pq}^{+[M,N]}(t,t')$, represents the scattering process $a_q^{\dagger}|N\rangle \to a_p^{\dagger}|M\rangle$, while the retarded-hole part, $G_{pq}^{-[M,N]}(t,t')$, accounts for ionization. For closed-shell targets, that is for $N = M = 0$, the OSGF of equation (3) boils down to the standard GF in equation (1). We studied the equation-of-motion of $G_{pq}^{[M,N]}(t,t')$ using Zubarev's method [16]. The result enables us to connect the OSGF to a self-energy $\boldsymbol{\Sigma}(\omega)$ through a generalized Dyson equation

$$
\boldsymbol{G}(\omega) = \boldsymbol{G}^{(0)}(\omega) + \boldsymbol{G}^{(0)}(\omega)\boldsymbol{\Sigma}(\omega)\boldsymbol{G}(\omega). \tag{4}
$$

Here $\boldsymbol{G}^{(0)}(\omega)$ is computed without particle–particle interaction and is equal to the direct product $\mathbf{1} \otimes \boldsymbol{g}^{(0)}(\omega)$. The dimension of the unit matrix, $\mathbf{1}$, is that of the degenerate manifold. The self-energy $\boldsymbol{\Sigma}(\omega)$ takes on the *same* appealing structure as that of the elastic one: $\Sigma_{pq}^{[M,N]}(\omega) = \Sigma_{pq}^{[M,N]}(\infty) + M_{pq}^{[M,N]}(\omega)$. The static term is given by $\Sigma_{pq}^{[M,N]}(\infty) = W_{pq}\delta_{MN} + \sum_{n,l}(V_{pnql} - V_{pnlq})\langle M|a_n^{\dagger}a_l|N\rangle$. Here $\boldsymbol{W}$ and $\boldsymbol{V}$ are the one- and two-body parts of the original interaction potential, respectively. The second and third terms are, respectively, the electrostatic and exchange interactions of the projectile with the exact one-particle densities of the target. Of course, if the projectile is distinguishable from the particles comprising the target, the exchange term vanishes identically. The dynamical term, $M_{pq}^{[M,N]}(\omega)$, couples all states in the degenerate manifold via a generalized response function. Its properties will be discussed elsewhere.

To show that $\boldsymbol{\Sigma}(\omega)$ is an OP for the various scattering processes $a_q^{\dagger}|N\rangle \to a_p^{\dagger}|M\rangle$ we recall that the corresponding multichannel S-matrix is given by $S_{pq}^{[M,N]} = {}^{-}\langle pM|qN\rangle^{+}$ [17]. The incoming and outgoing scattering states $|pM\rangle^{\pm}$ can be expressed using creation operators as $|pM\rangle^{\pm} = \lim_{t\to\mp\infty}\exp[-\mathrm{i}\varepsilon_p t]a_p^{\dagger}(t)|M\rangle$, where $\varepsilon_p = \frac{p^2}{2m}$ is the energy of the projectile [18]. It is now possible to relate $S_{pq}^{[M,N]}$ to $G_{pq}^{[M,N]}(t,t')$, namely,

$$
S_{pq}^{[M,N]} = \mathrm{i}\lim_{\substack{t\to+\infty\\ t'\to-\infty}} \mathrm{e}^{+\mathrm{i}\varepsilon_p t} G_{pq}^{+[M,N]}(t,t')\mathrm{e}^{-\mathrm{i}\varepsilon_q t'} = \mathrm{i}\lim_{\substack{t\to+\infty\\ t'\to-\infty}} \mathrm{e}^{+\mathrm{i}\varepsilon_p t} G_{pq}^{[M,N]}(t,t')\mathrm{e}^{-\mathrm{i}\varepsilon_q t'}. \tag{5}
$$

The last step in equation (5) is valid since the retarded-hole part, $G_{pq}^{-[M,N]}(t,t')$, vanishes identically for $t > t'$.

To proceed we break up the generalized Dyson equation (4) into two equations:

$$
\begin{aligned}
\boldsymbol{G}(\omega) &= \boldsymbol{G}^{(0)}(\omega) + \boldsymbol{G}^{(0)}(\omega)\boldsymbol{T}(\omega)\boldsymbol{G}^{(0)}(\omega), \\
\boldsymbol{T}(\omega) &= \boldsymbol{\Sigma}(\omega) + \boldsymbol{\Sigma}(\omega)\boldsymbol{G}^{(0)}(\omega)\boldsymbol{T}(\omega).
\end{aligned} \tag{6}
$$

Comparing equation (6) to its elastic counterpart, we find that $\boldsymbol{T}(\omega)$ plays the role of an improper self-energy. With the help of equation (6) one finds the final expression for the S-matrix:

$$
S_{pq}^{[M,N]}(\varepsilon_p) = \delta_{pq}\delta_{MN} - 2\pi\mathrm{i}T_{pq}^{[M,N]}(\varepsilon_p)\delta(\varepsilon_p - \varepsilon_q). \tag{7}
$$

Equation (7) reminds one of the text-book equation connecting the S-matrix to the T-matrix [17]. We have thus proven that the matrix $\boldsymbol{T}(\omega)$ defined in equation (6) is nothing but the (energetically-elastic) multichannel T-matrix. Following standard scattering theory we see from the relation (6) that $\boldsymbol{\Sigma}(\omega)$ is a potential governing the scattering process. Of course, both polarized (i.e. state-specific) and unpolarized energy-dependent cross sections can be calculated from the elements of $\boldsymbol{T}(\omega)$.

It is important to note that the above construction of $\boldsymbol{\Sigma}(\omega)$ does not restrict the nature of the degenerate states. In particular, these states do not need to correlate to single Slater determinants in the absence of particle–particle interaction. Like the text-book OP, $\mathbf{\Sigma}(\omega)$ is a *one-particle* potential, which is Hermitian and non-singular at projectile energies below the first inelastic threshold. Finally, we note that our formulation applies to spatial and spin degeneracy (or any other type of degeneracy).

So far, we have used *only* the degeneracy property of the ground state manifold in order to construct the OP $\mathbf{\Sigma}(\omega)$. Consequently, $\mathbf{\Sigma}(\omega)$ describes *multichannel* scattering processes within the degenerate manifold. Having in mind that the many-body Hamiltonian is invariant under a specific *symmetry group*, and, hence, the states in the degenerate manifold are interrelated by symmetry operations, we can *further* reduce the above-obtained OP. In what follows we treat explicitly the case of spin degeneracy and a spin-$\frac{1}{2}$ projectile. We would like to stress that the symmetry analysis performed does not depend on the symmetry group of the many-body Hamiltonian.

Let the spin of the target in its ground state be S. The ground state manifold is denoted by $\{|M\rangle, M = S, \ldots, -S\}$. In the single-particle annihilation and creation operators we separate the spatial and spin degrees of freedom: $a_{p\sigma}(t)$ and $a^{\dagger}_{p\sigma}(t)$, where σ can assume two values—α (up) and β (down). By utilizing the Wigner–Eckart theorem we express the OSGF through the $[S, S]$ diagonal blocks $\mathcal{G}^{\sigma}_{pq} \equiv G^{[S,S]}_{p\sigma,q\sigma}$, which depend on the spatial one-particle indices. The reason for choosing the highest-multiplicity block, $M = S$, will be clarified below. The result takes on the following simple appearance:

$$\boldsymbol{G}(\omega) = \boldsymbol{A} \otimes [\mathcal{G}^{\alpha}(\omega) - \mathcal{G}^{\beta}(\omega)] + \mathbf{1} \otimes \mathcal{G}^{\beta}(\omega). \tag{8a}$$

Note that for $S = 0$ one has $\mathcal{G}^{\alpha}(\omega) = \mathcal{G}^{\beta}(\omega)$ and the familiar decomposition of the standard GF in case of spin-independent potentials is recovered [11]. The indices of the coefficient matrix $\boldsymbol{A}$ depend on the projectile and target spin variables only, hence its dimension is $2(2S + 1)$. The elements of $\boldsymbol{A}$, composed of products of $3j$-symbol terms $C^{j_1,j_2,j_3}_{m_1,m_2,m_3}$, are given by

$$A^{M,M'}_{\sigma,\sigma'} = (-1)^{-\sigma'+S-M+\frac{1}{2}} \sum_{\rho=0}^{1} (2\rho + 1) C^{\frac{1}{2},\frac{1}{2},\rho}_{-\sigma,\sigma',\sigma-\sigma'} \left(C^{S,S,\rho}_{S,-S,0}\right)^{-1} C^{S,S,\rho}_{M',-M,\sigma'-\sigma} C^{\frac{1}{2},\frac{1}{2},\rho}_{-\frac{1}{2},\frac{1}{2},0}. \tag{8b}$$

From equation (8b) one can verify that $\boldsymbol{A}$ is a symmetric and real matrix (due to the spin-independent particle–particle interaction). The simple structure of $\boldsymbol{A}$ allows one to diagonalize it and, hence, block diagonalize $\boldsymbol{G}(\omega)$ in equation (8). Only two distinct blocks

$$\mathcal{G}^{S+1/2}(\omega) = \mathcal{G}^{\alpha}(\omega), \qquad \mathcal{G}^{S-1/2}(\omega) = \frac{2S+1}{2S} \mathcal{G}^{\beta}(\omega) - \frac{1}{2S} \mathcal{G}^{\alpha}(\omega), \tag{9}$$

with the corresponding multiplicities of $2(S + 1)$ and $2S$, appear. This outcome suggests a transparent physical meaning: the GFs $\mathcal{G}^{S\pm 1/2}(\omega)$ describe scattering in many-particle states of total spin $S \pm 1/2$, where the corresponding multiplicities are just the usual magnetic multiplicities given by $2(S + 1)$ and $2S$, respectively. In proving this claim we have to examine the structure of the advanced-particle and retarded-hole parts of $\boldsymbol{G}(t, t')$. The advanced-particle part, $\boldsymbol{G}^{+}(t, t')$, can be expressed, suppressing a factor of $-\mathrm{i}$, as a *multiplication* of column and row vectors:

$$[a^{\dagger}_{p\sigma}(t)|S\rangle \ldots a^{\dagger}_{p\sigma}(t)|-S\rangle]^{\dagger} \times [a^{\dagger}_{q\sigma'}(t')|S\rangle \ldots a^{\dagger}_{q\sigma'}(t')|-S\rangle].$$

The components of these vectors are $(N + 1)$-particle states describing the addition of two spins: the spin-$\frac{1}{2}$ projectile and spin-S composite target. Therefore, block diagonalization of $\boldsymbol{G}^{+}(t, t')$ simply means going from a basis of two independent spins to the basis where their total spin is a good quantum number (we use the term spin-irreducible). In other words, autocorrelations of the spin-irreducible $(N + 1)$-particle states

$$|S \pm 1/2, m\rangle_q \equiv \sqrt{\frac{S + 1/2 \pm m}{2S + 1}}\, a^{\dagger}_{q\alpha}|m - 1/2\rangle \pm \sqrt{\frac{S + 1/2 \mp m}{2S + 1}}\, a^{\dagger}_{q\beta}|m + 1/2\rangle \tag{10}$$

$(-S \mp 1/2 \leqslant m \leqslant S \pm 1/2)$ give the block-diagonalized $\boldsymbol{G}^{+}(t,t')$. Interestingly, the same transformation which block diagonalizes $\boldsymbol{G}^{+}(t,t')$ also block diagonalizes $\boldsymbol{G}^{-}(t,t')$ and, hence, $\boldsymbol{G}(t,t')$. The reason is that the application of the Wigner–Eckart theorem (see equation (8)) yields the same result for *any* time-ordering of the annihilation and creation operators. This proves our claim that the block-diagonalized OSGF (see equation (9)) represents spin-irreducible, $(N+1)$-particle, *scattering* states.

Having determined that the GFs $\mathcal{G}^{S\pm 1/2}(\omega)$ in equation (9) correspond to spin-irreducible *scattering* states we would like to inquire whether there are OPs for these scattering channels *alone*. The answer is positive. Owing to the structure of the generalized Dyson equation (4), one can block diagonalize $\boldsymbol{\Sigma}(\omega)$ to give the spin-irreducible self-energies $\Sigma^{S\pm 1/2}(\omega)$, by utilizing the same transformation employed to block diagonalize $\boldsymbol{G}(\omega)$. Similarly, the same holds for the S-matrix and $\boldsymbol{T}(\omega)$ (see equations (5)–(7)) which block diagonalize into their spin-irreducible components $\mathcal{S}^{S\pm 1/2}$ and $\mathcal{T}^{S\pm 1/2}(\omega)$. Consequently, to each of the spin-irreducible *scattering* channels represented by $\mathcal{G}^{S\pm 1/2}(\omega)$ there is an *exact* spin-irreducible OP: $\Sigma^{S\pm 1/2}(\omega)$. We note that the spin-irreducible OPs are *independent* of the azimuthal quantum number (within each total spin manifold) as it should be for spin-independent interactions. Moreover, since the spin-irreducible scattering channels do not couple due to symmetry restrictions, the corresponding spin-irreducible OPs are *all* Hermitian below the inelastic thresholds. The latter correspond to the first $(N+1)$-particle, spin-irreducible, excited states. This result gives the spin-irreducible OPs of the OSGF the same role played by $\boldsymbol{\sigma}(\omega)$ for $\boldsymbol{g}(\omega)$.

All elastic scattering differential cross sections can be computed by utilizing the OPs found above. On the one hand, in scattering of unpolarized projectiles from unpolarized targets the (average) cross section depends on the weighted sum of the spin-irreducible transition probabilities. Spin-flip cross sections, on the other hand, can be expressed from the difference between spin-irreducible transition amplitudes [17]. The spin-irreducible transition amplitudes, $\mathcal{T}^{S\pm 1/2}(\omega)$, can be calculated from the spin-irreducible OPs, $\Sigma^{S\pm 1/2}(\omega)$, through the usual relations in equation (6) expressed for the single-channel quantities. This allows us to calculate spin-flip and average cross sections from the spin-irreducible OPs, $\Sigma^{S\pm 1/2}(\omega)$.

So far, we have discussed the existence and properties of the spin-irreducible OPs for scattering from open-shell targets. For some relevant cases they can be systematically *evaluated* by the *usual* diagrammatic analysis, as utilized for the text-book proper self-energy $\boldsymbol{\sigma}(\omega)$ [11]. Generally, in the absence of particle–particle interaction a member $|M\rangle$ of the degenerate manifold correlates to a linear combination of Slater determinants. Consequently, the diagrammatic approach for calculating the corresponding self-energy via Wick's theorem [11] breaks down. Fortunately, for most atomic and molecular systems there are genuine one-particle configurations within the *unperturbed* degenerate manifold. Due to Hund's rule, for example, the states with maximal/minimal magnetic quantum number, $|M=\pm S\rangle$, correspond to a *single* Slater determinant whenever spin–orbit and spin–spin couplings are neglected. For these cases, we can write a single-channel Dyson equation to each of the blocks $\mathcal{G}^{\sigma}(\omega)$, namely $\mathcal{G}^{\alpha,\beta}(\omega) = \mathcal{G}^{(0)}(\omega) + \mathcal{G}^{(0)}(\omega)\Sigma^{\alpha,\beta}(\omega)\mathcal{G}^{\alpha,\beta}(\omega)$, where $\mathcal{G}^{(0)}(\omega)$ is computed without particle–particle interaction. This allows us to express the spin-irreducible OPs, $\Sigma^{S\pm 1/2}(\omega)$, directly by the self-energies $\Sigma^{\alpha,\beta}(\omega)$. The result reads,

$$\Sigma^{S+1/2}(\omega) = \Sigma^{\alpha}, \qquad \Sigma^{S-1/2}(\omega) = \mathcal{G}^{(0)^{-1}} - 2S\left(\frac{2S+1}{\mathcal{G}^{(0)^{-1}} - \Sigma^{\beta}} - \frac{1}{\mathcal{G}^{(0)^{-1}} - \Sigma^{\alpha}}\right)^{-1}. \quad (11)$$

The self-energies $\Sigma^{\alpha,\beta}(\omega)$ can be systematically evaluated by the *usual* diagrammatic analysis [14] and, subsequently, the spin-irreducible OPs $\Sigma^{S\pm 1/2}(\omega)$ can be calculated via equation (11).

One may argue why one should not use the self-energies $\Sigma^{\alpha,\beta}(\omega)$ instead of the spin-irreducible OPs $\Sigma^{S\pm1/2}(\omega)$ to calculate cross sections. Indeed, $\Sigma^{\alpha}(\omega)$ is a Hermitian and well-behaved function. Unfortunately, the self-energy $\Sigma^{\beta}(\omega)$ is a non-Hermitian potential and on top of that exhibits a cut starting already at zero energy. This can readily be understood by noticing that $\Sigma^{\beta}(\omega)$ accounts for the spin-flip process $a^{\dagger}_{q\beta}|S\rangle \rightarrow a^{\dagger}_{p\alpha}|S-1\rangle$, which is an open channel for any projectile energy. Consequently, the usage of $\Sigma^{\beta}(\omega)$ as an OP *by itself* is hardly practical. Fortunately, the symmetry arguments described above dictate that the spin-irreducible OPs are Hermitian and well-behaved functions and therefore are practical tools for scattering calculations. For the spin-irreducible OP $\Sigma^{S-1/2}(\omega)$ this is achieved by the coupling of both $\Sigma^{\alpha,\beta}(\omega)$ (see equation (11)) which *shifts* the singular properties of $\Sigma^{\beta}(\omega)$ to the *inelastic* threshold. This puts the scattering of electrons from open-shell atoms and molecules on a firm theoretical foundation, similarly to that possessed by scattering from closed-shell targets.

In conclusion, the OSGF has been introduced in order to tackle the problem of scattering from open-shell targets. The self-energy of the OSGF has been shown to be an *exact* OP for scattering from the degenerate ground state. By doing so, we reduced the many-body problem of scattering from open-shell targets to the scattering of a projectile by an *exact* one-body potential. Moreover, it has been shown that *exact* OPs can be constructed for specific elastic processes within the degenerate manifold, for example, for spin-flip processes. Taking into account the symmetry of the many-body Hamiltonian, spin-irreducible (in general, symmetry-irreducible) OPs have been shown to be the analogues of the usual self-energy. In particular, they exhibit similar analytic properties and, for most atomic and molecular systems, can be evaluated through Feynman's diagrams. Our results open the door to treating the very intricate scattering processes from open-shell targets with tools as attractive and common as used for closed-shell targets.

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References

[1] Lee K *et al* 1993 *Phys. Rev. Lett.* **70** 738
Viviani M *et al* 2001 *Phys. Rev. Lett.* **86** 3739
[2] Sakaguchi H *et al* 1982 *Phys. Rev.* C **26** 944
Kato S *et al* 1985 *Phys. Rev.* C **31** 1616
Ibaraki M *et al* 2000 *Nucl. Instrum. Methods Phys. Res.* A **446** 538
[3] Baum G *et al* 1999 *Phys. Rev. Lett.* **82** 1128
Meintrup R *et al* 2000 *J. Phys. B: At. Mol. Opt. Phys.* **33** L289
[4] Hegemann T *et al* 1991 *Phys. Rev. Lett.* **66** 2968
[5] Greenwood J B *et al* 1995 *Phys. Rev. Lett.* **75** 1062
[6] da Paixão F J *et al* 1992 *Phys. Rev. Lett.* **68** 1698
[7] Capuzzi F and Mahaux C 1995 *Ann. Phys., NY* **239** 57
[8] Michel F and Reidemeister G 1996 *Phys. Rev.* C **53** 3032
[9] Feshbach H 1962 *Ann. Phys., NY* **19** 287
[10] Bell J S and Squires E J 1959 *Phys. Rev. Lett.* **3** 96
[11] Fetter A L and Walecka J D 1971 *Quantum Theory of Many-Particle Systems* (New York: McGraw-Hill)
[12] Kerman A K, McManus H and Thaler R M 1959 *Ann. Phys., NY* **8** 551
[13] Layzer A J 1963 *Phys. Rev.* **129** 897
[14] Cederbaum L S and Schirmer J 1974 *Z. Phys.* **271** 221
[15] Cederbaum L S 2000 *Phys. Rev. Lett.* **85** 3072
Cederbaum L S 2001 *Ann. Phys., NY* **291** 169
[16] Zubarev D N 1960 *Sov. Phys.–Usp.* **3** 320
[17] Bransden B H 1983 *Atomic Collision Theory* (London: Benjamin)
[18] Csanak G *et al* 1971 *Adv. At. Mol. Phys.* **7** 287