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A many-body treatment of Feshbach theory applied to electron-atom and electron-molecule collisions*

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The Feshbach projection-operator technique is investigated using second quantization to construct approximate optical potentials with Tamm-Dancoff–approximation and random-phase–approximation descriptions for closed-shell targets. We interpret a recent many-body theory of elastic scattering (due to Schneider, Taylor, and Yaris) as an approximate form of the equations of this work. Possible applications and extensions of the method are also described.

I. INTRODUCTION

The optical model,[1] which provides a formal method for reducing a many-channel scattering problem to an equivalent one-body problem, has proven to be an effective device in the study of low-energy electron-atom scattering. There are several approaches which have been used to formulate the optical-model potential.

Because of its conceptual elegance and complete generality, Feshbach's theory of nuclear reactions[2] has been applied extensively to the study of atomic problems. Quite frequently however, Feshbach's projection-operator formalism serves more as an interpretive tool than a computational one. Indeed, almost all of the *numerical* applications of Feshbach theory have been restricted to two-electron systems, where the required projection can be constructed exactly.[3] The formulation lends itself most directly to the study of compound resonance states,[4] and it is certainly in this context that most applications have been made, although there have been a number of successful attempts to construct a Feshbach optical potential and use it to obtain nonresonant cross sections as well.[5]

Another approach to the optical model has been used which does not require the construction of projection operators and which can be systematically applied to larger systems. This approach is based on the fact that the proper self-energy of the one-particle Green's function of many-body theory can also serve as an elastic optical potential.[6] The self-energy can be approximated using the diagrammatic techniques of many-body perturbation theory.[7] Alternatively, Schneider, Taylor, and Yaris[8] have developed a nonperturbative approximation scheme for calculating the self-energy based on the Martin-Schwinger Green's-function theory.[9] This approach has met with great quantitative success in describing low-energy e^--helium scattering.[10]

In this paper, we show how the equations-of-motion technique[11] can be used to construct an approximate optical potential which describes the elastic scattering of an electron by a closed-shell atom or molecule. The problem is formulated in the language of second quantization, which is most convenient when discussing systems of identical fermions. Rather than working with the proper self-energy, however, we develop our approximation scheme in the Feshbach projection-operator formalism. We will also be able to show how an approximate optical potential, quite similar to the one derived by Schneider, Taylor, and Yaris[8] (hereafter referred to as STY) follows naturally from the equations-of-motion approach to Feshbach theory.

In the section that follows we derive the optical-model potential at two levels of approximation, first in the Tamm-Dancoff approximation (TDA),[11a] which ignores correlation in the target ground state, and then in the random phase approximation[11] (RPA), which implicitly includes some effects of target correlations. In Sec. III we compare the results of STY with those obtained here, and Sec. IV contains a brief summary and a conclusion.

II. THEORY

A. TDA description of target

Feshbach theory calls for the construction of an operator P which projects out the parts of the exact wave function that describe elastic scattering; that is, if ψ denotes the full wave function for the electron-atom (molecule) system, then P must satisfy the requirement that

$$P\psi \to \mathcal{A}F_0(r)\Phi_0(\{r_i\}), \tag{1}$$

where $\Phi_0(\{r_i\})$ is the ground-state wave function of the target and $F_0(r)$, the optical-model wave function, gives the correct elastic scattering. In addition to the projection operator P, we also require its orthogonal complement Q. An effective

Hamiltonian can then be constructed which describes elastic scattering[2]:

$$(H_{\text{eff}} - E)P\psi = 0, \tag{2}$$

where

$$H_{\text{eff}} = PHP + PHQ[1/Q(E - H + i\eta)Q]QHP. \tag{3}$$

In this section we will discuss a model obtained by making a number of simplifying assumptions. We first assume that the closed-shell target ground state is well represented by the Hartree-Fock ground-state wave function and that the excited states of the target may be described by the TDA. Introducing the creation and annihilation operators $a_p^\dagger$ and a_p referring to the particle states ϕ_p of the Hartree-Fock Hamiltonian, we may formulate the model as follows.

The operators P and Q are chosen as

$$P = \sum_p a_p^\dagger |\text{HF}\rangle\langle\text{HF}| a_p, \tag{4}$$

$$Q = \sum_{pp'} \sum_{\lambda\lambda'} a_p^\dagger |\lambda\rangle S^{-1}_{p\lambda,p'\lambda'} \langle\lambda'| a_{p'}, \tag{5}$$

where $|\text{HF}\rangle$ is the HF ground state and $|\lambda\rangle$ is an excited TDA target state which is generated by the TDA excitation operator $O_\lambda^\dagger$,

$$|\lambda\rangle = O_\lambda^\dagger |\text{HF}\rangle, \tag{6}$$

$$O_\lambda^\dagger = \sum_{m\alpha} X_{m\alpha}(\lambda) a_m^\dagger a_\alpha. \tag{7}$$

m and α denote particle and hole states, respectively, and the $X_{m\alpha}(\lambda)$'s are TDA amplitudes which satisfy the orthogonality condition

$$\sum_{m\alpha} X^*_{m\alpha}(\lambda) X_{m\alpha}(\lambda) = \delta_{\lambda\lambda'}. \tag{8}$$

In Eq. (5), $S^{-1}_{p\lambda,p'\lambda'}$ is an element of the inverse of the overlap matrix $S_{p\lambda,p'\lambda'}$,

$$S_{p\lambda,p'\lambda'} = \langle\text{HF}| O_\lambda a_p a_{p'}^\dagger O_{\lambda'}^\dagger |\text{HF}\rangle$$
$$= \delta_{pp'}\delta_{\lambda\lambda'} - \sum_\alpha X^*_{p'\alpha}(\lambda) X_{p\alpha}(\lambda'). \tag{9}$$

With these restrictions, it is easy to verify that P and Q are indeed projection operators and that they satisfy the necessary conditions $PQ = QP = 0$ and $P + Q = 1$ within the space of vectors spanned by the set $a_p^\dagger|\text{HF}\rangle$, $a_p^\dagger|\lambda\rangle$. This implies that $P\psi$ has the form

$$P\psi = \sum_p C_p a_p^\dagger |\text{HF}\rangle, \tag{10}$$

which is consistent with Eq. (1) and our assumptions about the target.

It may help to conceptualize the above approximations if we draw an analogy between the present scheme and a conventional close-coupling approximation, in which TDA target states are used for the expansion and the various channel wave functions are all expanded in terms of Hartree-Fock particle orbitals.

We now discuss the construction of the operators in Eq. (3) with the above choice of projectors P and Q. The Hamiltonian may be written in second quantization as[12]

$$H = \sum_i \epsilon_i :a_i^\dagger a_i: + \tfrac{1}{2} \sum_{ijkl} V_{ijkl} :a_i^\dagger a_j^\dagger a_l a_k:, \tag{11}$$

where sums on i, j, k, and l go over hole and particle states (spin orbitals), V_{ijkl} is given by

$$V_{ijkl} = \int \phi_i^*(r_1)\phi_j^*(r_2) \frac{1}{|r_1 - r_2|} \phi_k(r_1)\phi_l(r_2)\, d^3r_1\, d^3r_2, \tag{12}$$

ϵ_i is a Hartree-Fock orbital energy, and the operators are normal ordered with respect to the HF ground state. The Hartree-Fock ground-state energy has been chosen as the zero of energy and has thus been subtracted from the Hamiltonian.

The operators PHP and PHQ may be formed easily from the above definitions. Repeated application of Wick's theorem to the matrix elements involved yields for H_{pp}

$$H_{pp} = \sum_p a_p^\dagger |\text{HF}\rangle \epsilon_p \langle\text{HF}| a_p. \tag{13}$$

If we define antisymmetrized matrix elements $\tilde{V}_{ijkl}$ by

$$\tilde{V}_{ijkl} = V_{ijkl} - V_{ijlk}, \tag{14}$$

the result for PHQ is

$$PHQ = \sum_{pqp'} \sum_{\lambda\lambda'} \sum_{m\gamma} a_p^\dagger |\text{HF}\rangle X_{m\alpha}(\lambda) \tilde{V}_{\alpha pmq} \times S^{-1}_{\lambda q,\lambda' p'} \langle\text{HF}| O_{\lambda'} a_{p'}. \tag{15}$$

In Eq. (15) sums on p, p', q, and m are over particle states, and the sum on γ is over hole states.

The form of $Q(E - H)Q$ is more complicated and is given in the appendix. To complete the present approximation consistently, one should diagonalize QHQ in the (nonorthogonal) basis $\{a_p^\dagger|\lambda\rangle\}$ and then construct H_{eff} via Eq. (3). However we may develop a diagonal approximation as follows. The matrix element involved in $Q(E - H)Q$ is

$$\langle\text{HF}| O_\lambda a_p (E - H) a_{p'}^\dagger O_{\lambda'}^\dagger |\text{HF}\rangle.$$

Following a similar argument by Dietrich and Hara,[12] we assume that the states formed by adding a particle to the TDA description of the excited target are eigenfunctions of the full Hamiltonian,

$$H a_p^\dagger O_\lambda^\dagger |\text{HF}\rangle = (\epsilon_p + \omega_\lambda) a_p^\dagger O_\lambda^\dagger |\text{HF}\rangle,$$

where ω_λ is the TDA excitation energy (recall that the zero of energy has been defined as $E_{\rm HF}$). With this approximation the matrix element above becomes

$$\langle \mathrm{HF}|O_\lambda a_p (E-H) a_{p'}^\dagger O_{\lambda'}^\dagger|\mathrm{HF}\rangle = (E-\omega_\lambda-\epsilon_p)S_{\lambda p,\lambda' p'}. \tag{16}$$

Further, assuming $S_{\lambda p,\lambda' p'}=\delta_{\lambda\lambda'}\delta_{pp'}$ we obtain an approximate form of the optical potential:

$$H_{\rm eff}=\sum_p a_p^\dagger|\mathrm{HF}\rangle\epsilon_p\langle\mathrm{HF}|a_p+\sum_{pp'}\sum_{q\lambda}\sum_{mn}\sum_{\gamma\sigma}\frac{a_p^\dagger|\mathrm{HF}\rangle X_{m\gamma}(\lambda)X_{n\sigma}^*(\lambda)\tilde{V}_{\gamma pmq}\tilde{V}_{nq\sigma p'}\langle\mathrm{HF}|a_{p'}}{E-\omega_\lambda-\epsilon_p+i\eta}. \tag{17}$$

This expression for $H_{\rm eff}$ has the analytic structure one would expect from the exact Feshbach optical potential, namely branch cuts formed by the set of continuous energies ϵ_q, one such cut associated with each inelastic threshold labeled by the ω_λ's. However, $H_{\rm eff}$ does not possess the isolated poles associated with the resonance states of the compound system which were lost when neglecting the off-diagonal pieces of QHQ.

B. RPA description of target

One can go beyond the TDA description used in Sec. II A and implicitly include some of the effects of correlation in the target. In this section, we outline a method for approximating $H_{\rm eff}$ in the random phase approximation (RPA).[11] If $|0\rangle$ denotes the ground state of the target, then excited states $|\lambda\rangle$ are generated by the RPA excitation operator $O_\lambda^\dagger$,

$$|\lambda\rangle = O_\lambda^\dagger|0\rangle, \tag{18}$$

where

$$O_\lambda^\dagger=\sum_{m\alpha}[Y_{m\alpha}(\lambda)a_m^\dagger a_\alpha - Z_{m\alpha}(\lambda)a_\alpha^\dagger a_m] \tag{19}$$

and the sums on m and α run over particle-hole pairs.

Consider the projection operators

$$P=\sum_{pp'}a_p^\dagger|0\rangle M_{pp'}^{-1}\langle 0|a_{p'}, \tag{20a}$$

$$Q=\sum_{pp'}\sum_{\lambda\lambda'}a_p^\dagger O_\lambda^\dagger|0\rangle S_{\lambda p,\lambda' p'}^{-1}\langle 0|O_{\lambda'}a_{p'}, \tag{20b}$$

where

$$M_{pp'}=\langle 0|a_p a_{p'}^\dagger|0\rangle, \tag{21a}$$

$$S_{\lambda p,\lambda' p'}=\langle 0|O_\lambda a_p a_{p'}^\dagger O_{\lambda'}^\dagger|0\rangle. \tag{21b}$$

To verify that PQ is still zero, we must consider a matrix element of the form

$$\langle 0|a_p a_{p'}^\dagger O_\lambda^\dagger|0\rangle.$$

Following Shibuya and McKoy,[11] we retain terms in $|0\rangle$ through first order in the correlation coefficients $C_{mn}^{\alpha\beta}$:

$$|0\rangle\approx N_0\left(1+\sum_{m\alpha}\sum_{n\beta}C_{mn}^{\alpha\beta}a_m^\dagger a_n^\dagger a_\alpha a_\beta\right)|\mathrm{HF}\rangle. \tag{22}$$

With this choice for $|0\rangle$, it follows that the matrix element $\langle 0|a_p a_{p'}^\dagger O_\lambda^\dagger|0\rangle$ is zero and that the choices for P and Q are valid.

In discussing the RPA, we are faced with a problem that was not present when the TDA was used. The ground state $|0\rangle$ is assumed to be correlated, yet the RPA equations that are solved for the excitation operators $O_\lambda^\dagger$ do not specify the correlation coefficients. If the correlation coefficients in Eq. (22) are known (e.g., from Raleigh-Schrödinger perturbation theory), the effective Hamiltonian can be constructed in a straightforward manner from the definitions of P and Q—although the matrix elements involved will be quite complicated. In this section, however, we will take another approach more consistent with the derivation of the RPA. We will replace matrix elements of the form $\langle 0|A|0\rangle$ by equivalent commutator expressions which lower the particle rank of the operator A, and then approximate $|0\rangle$ by the Hartree-Fock ground state.

Consider PHQ which requires matrix elements of the form

$$\langle 0|a_p H a_{p'}^\dagger O_\lambda^\dagger|0\rangle.$$

If $O_\lambda^\dagger$ were an exact solution of the equations of motion for the excitation operator, we would have the identity

$$O_\lambda|0\rangle=0. \tag{23}$$

We apply this relation followed by the approximation $|0\rangle\approx|\mathrm{HF}\rangle$ to obtain

$$\begin{aligned}\langle 0|a_p H a_{p'}^\dagger O_\lambda^\dagger|0\rangle &= \langle 0|[a_p H a_{p'}^\dagger, O_\lambda^\dagger]|0\rangle \\ &\approx \langle \mathrm{HF}|[a_p H a_{p'}^\dagger, O_\lambda^\dagger]|\mathrm{HF}\rangle.\end{aligned} \tag{24}$$

With this approximation PHQ may be easily evaluated

$$\begin{aligned}PHQ=\sum_{pp'qq'}\sum_{\lambda\lambda' m\alpha}a_p^\dagger|0\rangle M_{pq}^{-1}\{&Y_{m\alpha}(\lambda)\tilde{V}_{q\alpha p' m} \\ &+Z_{m\alpha}(\lambda)\tilde{V}_{qmp'\alpha}\} \\ &\times S_{p'\lambda,q'\lambda'}^{-1}\langle 0|O_{\lambda'}a_{q'}.\end{aligned} \tag{25}$$

To complete the construction of the effective Hamiltonian in this approximation, we must evaluate the matrix elements of QHQ and diagonalize it. The matrix elements of QHQ are given in the ap-

pendix. In the spirit of Sec. IIA, we may again construct a diagonal approximation by following Dietrich and Hara[12] in assuming that states formed by adding an electron in an HF particle state to RPA excited states of the target are eigenfunctions of the full Hamiltonian,

$$Ha_p^\dagger O_\lambda^\dagger|0\rangle = (\omega_\lambda + \epsilon_p) a_p^\dagger O_\lambda^\dagger|0\rangle, \tag{26}$$

where ω_λ is the RPA excitation energy. We also assume $S_{\lambda p, \lambda' p'}$ is the unit matrix. To write an approximate effective Hamiltonian which can be constructed from the results of an RPA calculation on the target without knowledge of the correlation coefficients, we must replace $a_p^\dagger|0\rangle$ in Eqs. (20a) and (25) by $a_p^\dagger|\mathrm{HF}\rangle$ which makes $M_{pp'}$ the unit matrix and PHP the same operator used in the TDA derivation. With these assumptions the effective Hamiltonian is

$$H_{\mathrm{eff}} = \sum_p a_p^\dagger|\mathrm{HF}\rangle \epsilon_p \langle \mathrm{HF}|a_p + \sum_{pp'q\lambda} \sum_{m\gamma n\delta} a_p^\dagger|\mathrm{HF}\rangle \{Y_{m\gamma}(\lambda)\tilde{V}_{\gamma pmq} + Z_{m\gamma}(\lambda)\tilde{V}_{mp\gamma q}\} \times \frac{1}{E - \omega_\lambda - \epsilon_q + i\eta} \{Y^*_{n\delta}(\lambda)\tilde{V}_{nq\delta p'} + Z^*_{n\delta}(\lambda)\tilde{V}_{\delta qnp'}\}\langle \mathrm{HF}|a_{p'}. \tag{27}$$

III. COMPARISON WITH OTHER WORK

At this point, we will analyze the RPA effective Hamiltonian in its *approximate* diagonal form and point out the similarities and differences between this result and the expression derived by STY.

Equation (27) for H_{eff} is an operator expression which is valid in the subspace of $N+1$ particle vectors spanned by the set $a_p^\dagger|\mathrm{HF}\rangle$. It has the form

$$H_{\mathrm{eff}} = \sum_{pp'} a_p^\dagger|\mathrm{HF}\rangle H_{\mathrm{eff}}^{pp'} \langle \mathrm{HF}|a_{p'}. \tag{28}$$

We can identify $H_{\mathrm{eff}}^{pp'}$ as a matrix element of the effective one-body Hamiltonian H^{opt} that gives the optical-model wave function $F_0(r)$ and satisfies the equation

$$(E + \tfrac{1}{2}\nabla_r^2)F_0(r) = H^{\mathrm{opt}}(r, r')F(r'). \tag{29}$$

$H^{\mathrm{opt}}(r, r')$ is easily extracted from Eq. (27) as

$$H^{\mathrm{opt}}_{(r,r')} = V_{\mathrm{HF}}(r, r') + \sum_{m\gamma} \sum_{n\delta} \sum_{q\lambda} \{[Y_{m\gamma}(\lambda)V_{\gamma m}(r)\phi_q(r) + Z_{m\gamma}(\lambda)V_{m\gamma}(r)\phi_q(r)] - [Y_{m\gamma}(\lambda)V_{\gamma q}(r)\phi_m(r) + Z_{m\gamma}(\lambda)V_{mq}(r)\phi_\gamma(r)]\} \times \frac{1}{E - \omega_\lambda - \epsilon_q + i\eta} \{[Y^*_{n\delta}(\lambda)V_{q\delta}(r')\phi^*_q(r') + Z^*_{n\delta}(\lambda)V_{\delta n}(r')\phi^*_q(r')] - [Y^*_{n\delta}(\lambda)V_{q\delta}(r')\phi^*_n(r') + Z^*_{n\delta}(\lambda)V_{qn}(r')\phi^*_\delta(r')]\} \tag{30}$$

where the sums on m, n, and q run over particle states, the sums on γ and δ over hole states and

$$V_{ij}(r) \equiv \int \phi_i^*(r')\phi_j(r')(1/|r - r'|)\, d^3r'. \tag{31}$$

The Hartree-Fock potential $V_{\mathrm{HF}}(r, r')$ which came from PHP is

$$V_{\mathrm{HF}}(r, r') = \sum_n \frac{Z_n}{|R_n - r|}\delta(r - r') + \sum_\gamma [J_\gamma(r)\delta(r - r') - K_\gamma(r, r')], \tag{32}$$

where the first term gives the nuclear attraction and J_γ and K_γ are the usual Coulomb and exchange operators.

Equation (30) is essentially the same as the effective Hamiltonian derived by STY by approximating the proper self-energy of the one-particle Green's function with some minor differences which we now discuss. First the cut structure of Eq. (30) is the same as that of the TDA result of Eq. (17), i.e., branch cuts associated with each inelastic threshold. The STY result also has terms with energy denominators $(Z + \omega_\lambda - \epsilon_\mu)$ where ϵ_μ is a hole-state orbital energy. These terms give rise to discrete poles on the negative energy axis and a left-hand cut corresponding to the ionization continuum of the target. From the formal analytic structure of the proper self-energy,[13] it might be expected that such terms would appear in any approximation scheme. However the Feshbach optical potential has no singularities at negative energies (that is, negative with respect to the energy of the target ground state), and consequently no such singularities appear in our approximations. In any case we expect such terms to contribute negligibly to a scattering calculation, since at physical energies all such terms have large positive energy denominators. This supposition is verified by comparison of the results on e^--He scattering of Pu and Chang[5] with those of Yarlagadda, Csanak, Taylor, Schneider, and Yaris.[10]

A more serious discrepancy between our result and that of STY is that at energies at which both

optical potentials are real, the present result is symmetric in r and r' whereas the STY optical potential is not. Consequently the STY optical potential is non-Hermitian at all energies. If we use the terminology of STY, we can write Eq. (30) symbolically as

$$H_{\text{eff}} = V_{\text{HF}} + \frac{(W_{\text{direct}} - W_{\text{exchange}})(W^*_{\text{direct}} - W^*_{\text{exchange}})}{E - U} . \tag{33}$$

The STY result does not have the term W_{exchange}, and consequently is nonsymmetric, and does not couple triplet states of the target which only contribute to the term $W_{\text{exchange}} W^*_{\text{exchange}}/(E-U)$. This apparently did not have a serious effect on the e^--He elastic scattering computations of Yarlagadda *et al.*,[10] but for He, V_{HF} alone gives most of the elastic cross section.[14] This may not be the case for larger systems where the coupling to triplet target states might be more important. It has been kindly pointed out to us by Yarlagadda and Csanak that the non-Hermitian potential of STY results from a nonsymmetric choice of operators in their approximation scheme and may be remedied in several ways.[15]

We should also like to mention two recent studies on e^--He which bear some resemblance to the method proposed here. Temkin, Bhatia, and Bardsley[16] have proposed an optical-potential scheme and, considering the Q part of the problem only, successfully calculated the position and width of the lowest ^2S resonance of He^-. Murtaugh and Reinhardt,[14] using a method which they show to be equivalent to an approximate optical-potential calculation, obtained similar results for the resonance position and accurate nonresonant S-wave phase shifts as well. While neither of the above references make use of second quantization in developing their approximation, it would appear that both approaches bear a strong resemblance to the "nondiagonal" optical potential we have detailed in the appendix.[17]

IV. DISCUSSION

We have shown how to apply many-body techniques to the Feshbach projection-operator formalism and obtain consistent approximations to the optical potential for closed-shell target atoms and molecules in both the TDA and RPA. We have also interpreted the results of STY as a "diagonal" approximation to the equations we obtained and thus have shown why the STY optical potential is incapable of displaying resonance behavior. The form of H_{eff} given in Eq. (17) or Eq. (30) lends itself directly to numerical computation, although we reiterate that a more elaborate calculation that would also treat resonances properly could be carried out by diagonalizing QHQ as given in the appendix.

It has been shown by numerous authors that the optical potential, for purely elastic scattering, is well represented by a discrete-basis-set expansion which gives a finite pole representation. Thus H_{eff} as given by Eq. (30) can be formed from the results of finite basis set Hartree-Fock and RPA calculations on the target. Once the optical potential is formed, its use in a scattering calculation is no more difficult than the use of $V_{\text{HF}}(r, r')$, which is also a nonlocal operator. The present authors have recently shown that continuum HF calculations can be carried out for small molecules by using purely discrete basis-set techniques.[18] For applications to molecular systems the restriction to closed-shell targets is not a severe one since most small molecules of interest have closed-shell ground states.

For energies above the first inelastic threshold, the discrete pole approximation to H_{eff} is inappropriate as it stands. However in this case one could follow Nuttall[19] in performing the calculation at complex energies and obtain results at physical energies by extrapolation.

The techniques developed here can be extended to inelastic scattering by the inclusion of more than one channel in P. A similar technique has been used by Burke and Taylor[5] in calculations on e^--H scattering.[20] In a later paper we will pursue this course in developing a many-body approach to multichannel scattering.

APPENDIX: EXPLICIT FORMULAS FOR QHQ

The matrix elements of the Hamiltonian given in this appendix were generated using a computer program which automates the application of Wick's theorem for arbitrary operators. We are grateful to Danny L. Yeager for instructing us in the use of his program and for modifying it to suit our needs.

A. TDA target

$$QHQ = \sum_{pp'} \sum_{qq'} \sum_{\lambda\lambda'} \sum_{\chi''\lambda'''} a_p^\dagger O_\lambda^\dagger |\text{HF}\rangle S^{-1}_{p\lambda,q\chi} \times \langle \text{HF}| O_\chi a_q H a^\dagger_{q'} O^\dagger_{\chi''} |\text{HF}\rangle \times S^{-1}_{q'\chi'',p'\chi'''} \langle \text{HF}| O_{\chi'''} a_{p'},$$

where $O^\dagger_\lambda$ is the TDA excitation operator of Eq. (7), S is the overlap matrix of Eq. (9), and

$$\langle \mathrm{HF}|O_{\lambda'}\, a_q H a_{q'}^{\dagger}, O_{\lambda''}^{\dagger}|\mathrm{HF}\rangle = \sum_{m\alpha m'\alpha'} Y^{*}_{m\alpha}(\lambda')Y_{m'\alpha'}(\lambda'')[\delta_{\alpha\alpha'}\delta_{mm'}\delta_{qq'}(\epsilon_q+\epsilon_m-\epsilon_\alpha)-\delta_{\alpha\alpha'}\delta_{mq'}\delta_{m'q}(\epsilon_{m'}+\epsilon_m-\epsilon_\alpha)$$
$$+\delta_{qq'}\tilde{V}_{m\alpha'\alpha m'}+\delta_{pm'}\tilde{V}_{m\alpha' q'\alpha}+\delta_{q'm}\tilde{V}_{q\alpha' m'\alpha}+\delta_{mm'}\tilde{V}_{\alpha' qq'\alpha}$$
$$+\delta_{\alpha\alpha'}\tilde{V}_{mqm'q'}]. \tag{A1}$$

B. RPA target

$$QHQ=\sum_{pp'}\sum_{\lambda\lambda'}\sum_{\lambda''\lambda'''}\sum_{qq'} a_p^{\dagger}O_{\lambda}^{\dagger}|0\rangle S^{-1}_{p\lambda,q\lambda''}$$
$$\times\langle 0|O_{\lambda'}\, a_q H a_{q'}^{\dagger}, O_{\lambda''}^{\dagger}|0\rangle$$
$$\times S^{-1}_{q'\lambda'',p'\lambda'''}\langle 0|O_{\lambda'''}\, a_{p'},$$

where $O_\lambda^\dagger$ is the RPA excitation operator of Eq. (19) and $S^{-1}_{p\lambda,p'\lambda'}$ is an element of the inverse of the overlap matrix $S_{p\lambda,p'\lambda'}$ of Eq. (21b).

Consider a general matrix element of the form $\langle 0|O_\lambda A O_{\lambda'}^{\dagger}|0\rangle$. Using the property that $O_\lambda|0\rangle=0$, this matrix element can be written as

$$\langle 0|O_\lambda A O_{\lambda'}^{\dagger}|0\rangle=\langle 0|[O_\lambda, A, O_{\lambda'}^{\dagger}]|0\rangle$$
$$+\tfrac{1}{2}\langle 0|AO_\lambda O_{\lambda'}^{\dagger}|0\rangle$$
$$+\tfrac{1}{2}\langle 0|O_\lambda O_{\lambda'}^{\dagger}A|0\rangle, \tag{A2}$$

where the symmetric double commutator is defined by the relation

$$[A,B,C]=\tfrac{1}{2}[A,[B,C]]+\tfrac{1}{2}[[A,B],C].$$

In evaluating the above matrix element, we appeal to the same arguments used in Sec. II A of the text in replacing $|0\rangle$ by $|\mathrm{HF}\rangle$. We also assume, for the purpose of evaluating the last two terms of Eq. (A2), that O_λ and $O_{\lambda'}^{\dagger}$ are boson operators—the quasiboson approximation

$$[O_\lambda, O_{\lambda'}^{\dagger}]=\delta_{\lambda\lambda'},$$

so that

$$\langle 0|O_\lambda A O_{\lambda'}^{\dagger}|0\rangle\approx\langle \mathrm{HF}|[O_\lambda, A, O_{\lambda'}^{\dagger}]|\mathrm{HF}\rangle$$
$$+\delta_{\lambda\lambda'}\langle 0|A|0\rangle. \tag{A3}$$

Note that if $|0\rangle$ is expanded as in Eq. (22), then $\langle 0|A|0\rangle=\langle \mathrm{HF}|A|\mathrm{HF}\rangle$ plus terms of orders $(C_{mn}^{\alpha\beta})^2$ and $\tilde{V}_{\alpha\beta,pq}C_{mn}^{\alpha\beta}$ which we ignore. The results follow:

$$S_{p\lambda,p'\lambda'}=-\sum_{m'\alpha'}\sum_{m\alpha}\{Y_{m'\alpha'}(\lambda)Y^{*}_{m\alpha}(\lambda')\delta_{\alpha\alpha'}\delta_{mp'}\delta_{pm'}+Z_{m'\alpha'}(\lambda)Z^{*}_{m\alpha}(\lambda')\delta_{\alpha\alpha'}\delta_{mp}\delta_{m'p'}\}+\delta_{\lambda\lambda'}\delta_{pp'}, \tag{A4}$$

$$\langle\lambda|a_p H a_{p'}^{\dagger}|\lambda'\rangle=\delta_{pp'}\sum_{m\alpha}[Y^{*}_{m\alpha}(\lambda)Y_{m\alpha}(\lambda')+Z^{*}_{m\alpha}(\lambda)Z_{m\alpha}(\lambda')](\epsilon_m-\epsilon_\alpha)$$
$$+\sum_{m\alpha}\sum_{m'\alpha'}[Y^{*}_{m\alpha}(\lambda)Y_{m'\alpha'}(\lambda')+Z^{*}_{m'\alpha'}(\lambda)Z_{m\alpha}(\lambda')][\delta_{pp'}\tilde{V}_{m\alpha'\alpha m'}+\delta_{pm'}\tilde{V}_{m\alpha' p'\alpha}+\delta_{p'm}\tilde{V}_{p\alpha' m'\alpha}+\delta_{mm'}\tilde{V}_{\alpha' pp'\alpha}$$
$$+\delta_{\alpha\alpha'}\tilde{V}_{pmp'm'}-\delta_{\alpha\alpha'}\delta_{mp'}\delta_{m'p}(\epsilon_{m'}+\epsilon_m-\epsilon_\alpha)]$$
$$+\sum_{m\alpha}\sum_{m'\alpha'}Y^{*}_{m\alpha}(\lambda)Z_{m'\alpha'}(\lambda')(\delta_{p'm}\tilde{V}_{m'p\alpha\alpha'}+\delta_{p'm'}\tilde{V}_{pm\alpha\alpha'}+\delta_{pp'}\tilde{V}_{mm'\alpha\alpha'})$$
$$+\sum_{m\alpha}\sum_{m'\alpha'}Y_{m'\alpha'}(\lambda')Z^{*}_{m\alpha}(\lambda)(\delta_{pm'}\tilde{V}_{\alpha'\alpha mp'}+\delta_{pm}\tilde{V}_{\alpha'\alpha p'm'}\delta_{pp'}\tilde{V}_{\alpha'\alpha m'm})+\delta_{\lambda\lambda'}\delta_{pp'}\epsilon_p. \tag{A5}$$

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