Distorted-wave methods for electron capture in ion-atom collisions

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Distorted-wave methods for electron capture are discussed with emphasis on the surface term in the T matrix and on the properties of the associated integral equations. The surface term is generally nonvanishing if the distorted waves are sufficiently accurate to include parts of the considered physical process. Two examples are considered in detail. If distorted waves of the strong-potential Born-approximation (SPB) type are employed the surface term supplies the first-Born-approximation part of the T matrix. The surface term is shown to vanish in the continuum-distorted-wave (CDW) method. The integral kernel is in either case free of the dangerous disconnected terms discussed by Greider and Dodd but the CDW theory is peculiar in the sense that its first-order approximation (CDW1) excludes a specific on-shell portion of the double-scattering term that is closely connected with the classical Thomas process. The latter is described by the second-order term in the CDW series. The distorted-wave Born approximation with SPB waves is shown to be free of divergences. In the limit of asymmetric collisions the DWB suggests a modification of the SPB approximation to avoid the divergence problem recently identified by Dewangan and Eichler.

I. INTRODUCTION

In 1964, Cheshire[1] proposed the continuum-distorted-wave (CDW) method in the impact-parameter picture to calculate electron capture in a high-energy electron-capture collision between a bare nucleus and a one-electron atom,

$$P^{Z_P+}+T^{(Z_T-1)+}(1s)\rightarrow P^{(Z_P-1)+}(nlm)+T^{Z_T+}\ , \quad (1)$$

where Z_T (Z_P) denotes the charge of the target (projectile) nucleus. Since then, the first-order CDW approximation (CDW1) has proven to be fairly successful in describing experimental total cross sections over a wide range of collision velocities (v) and target-projectile combinations.[2] The CDW1 approximation has received particular attention because it is simple enough to provide the T-matrix element in analytical form for arbitrary hydrogenic final states.[3]

Recent investigations have displayed, however, several unsatisfactory features of the CDW1 approximation. Among these are a "dip" in the differential capture cross section at the critical angle θ_T for Thomas double scattering[4] and an order-of-magnitude overestimate of the capture cross section into Rydberg states[5] with large angular momenta. Based on a quantum-mechanical treatment it has recently been suggested[6,7] that the CDW1 approximation is not a consistent first-order approximation within the framework of the distorted-wave theory by virtue of leaving out an additional hitherto unrecognized surface term.

In this paper we analyze the general distorted-wave method for electron capture and find an equivalence between the distorted-wave contribution to the T matrix in the quantal treatment and the surface term appearing in the time-dependent t-matrix approach in the impact-parameter picture. Two examples are discussed in detail. In the first example we use distorted waves of the strong-potential Born (SPB) type[8,9] as in Refs. 6 and 7. It is shown that the surface term in the impact-parameter treatment in this case provides the B1 (first Born) part of the transition amplitude, in agreement with the fact that the B1 part of the T matrix in the quantal treatment[7] also is provided by the distortion. It is found that the distorted-wave Born (DWB) series corresponding to SPB waves in initial and final channels has good convergence properties since the corresponding integral kernel is a "switch generator" which excludes the appearance of subseries of disconnected diagrams. The first-order term in this series, i.e., the DWB approximation, is free of divergent terms. This is contrasted with the recently identified divergence in the SPB approximation, and a properly modified SPB approximation is derived from the DWB in the limit of asymmetric collisions. In the second example we discuss the CDW method. The surface term is seen to vanish in the impact-parameter form of the CDW approach and we demonstrate explicitly that the corresponding distorted-wave contribution in the quantal treatment vanishes because of asymptotic orthogonality of the CDW waves. In harmony with recent work by Crothers and McCann[10,11] it is found that the second-order term of the ordinary Born series (the double scattering term) is not adequately represented by the first-order term in the CDW series. The dip in the differential CDW1 cross section at the critical angle θ_T for Thomas double scattering is traced to the lack of the second-order term in the residual interactions.[10]

II. DISTORTED-WAVE THEORY FOR REARRANGEMENT

A. Quantum-mechanical formulation

Following standard argumentation[8] we ignore the internuclear potential and write the total Hamiltonian as

$$H = H_0 + V_T + V_P \ , \tag{2}$$

where H_0 is the kinetic energy operator of the three-body system and V_P (V_T) is the interaction between the transferred electron and the projectile (target) nucleus. In order to apply standard results from scattering theory it is assumed that Coulomb interaction potentials are appropriately screened. This implies that special care must be exerted with limiting procedures to avoid inconsistencies if properties of the Coulomb field are eventually exploited in the evaluation of matrix elements.[9]

The total Hamiltonian can be decomposed into entrance (i) and exit (f) channel Hamiltonians

$$\begin{aligned} H_i &= H_T = H_0 + V_T \ , \\ H_f &= H_P = H_0 + V_P \ , \end{aligned} \tag{3}$$

and corresponding channel perturbations

$$\begin{aligned} V_i &= V_P \ , \\ V_f &= V_T \ . \end{aligned} \tag{4}$$

The exact ingoing ($+$) and outgoing ($-$) scattering states are defined as solutions of the wave equation ($c = i$ or f)

$$|\Psi_c^{\pm}\rangle = \Omega_c^{\pm} |\Phi_c\rangle \ , \tag{5}$$

where $\Omega_c^{\pm}$ is the Møller operator

$$\Omega_c^{\pm} = 1 + G^{\pm}(E) V_c \tag{6}$$

acting on a channel state of energy E, $|\Phi_c\rangle = |\mathbf{K}_c, \phi_{c\alpha}\rangle$ where $\mathbf{K}_c$ represents the channel wave number and $\phi_{c,\alpha}$ represents the internal state with binding energy ϵ_α. The full Green's operator in Eq. (6) is given by

$$G^{\pm}(E) = (E - H \pm i\eta)^{-1} \ , \tag{7}$$

where $\eta = 0^+$.

The T matrix is given in either of two forms which are equivalent on the energy shell. For simplicity we concentrate on the post form

$$T_{if} = \langle \Phi_f | V_i | \Psi_i^{\pm} \rangle \ , \tag{8}$$

Using well-known operator identities Eq. (8) may be expressed in various equivalent forms. For later convenience we note that

$$T_{if} = \lim_{\eta \to 0^+} i\eta \langle \Phi_f | \Psi_i^{\pm} \rangle \tag{9}$$

on the energy shell.

The distorted-wave method is based on a partitioning of the channel perturbations into distortions U and residual interactions W,

$$V_c = U_c + W_c \ . \tag{10}$$

In general, the decomposition is different in the two channels and U and W are not required to be local or Hermitian. The distorted waves taking into account the channel distortions are given by

$$|\chi_c^{\pm}\rangle = \omega_c^{\pm} |\Phi_c\rangle \ , \tag{11}$$

where $\omega_c^{\pm}$ are the distorted-wave Møller operators

$$\omega_c^{\pm} = 1 + g_c^{\pm} U_c \tag{12}$$

and

$$g_c^{\pm} = [E - (H_c + U_c) \pm i\eta]^{-1} \ . \tag{13}$$

The T matrix on the energy shell can then be expressed in the following exact form:[12]

$$T_{if} = \langle \chi_f^- | W_f^{\dagger} | \Psi_i^+ \rangle + T_{if}^D \ , \tag{14}$$

where

$$T_{if}^D = \langle \chi_f^- | V_i - W_f^{\dagger} | \Phi_i \rangle \ . \tag{15}$$

Using the relation $V_i - W_f^{\dagger} = (H_f + U_f)^{\dagger} - H_i$ one finds[6] that the following relation is valid on the energy shell:

$$T_{if}^D = \lim_{\eta \to 0^+} (i\eta \langle \chi_f^- | \Phi_i \rangle) \ . \tag{16}$$

This term clearly vanishes if χ_f^- is asymptotically orthogonal to Φ_i, i.e., if $\langle \chi_f^- | \Phi_i \rangle$ is bounded. According to Eq. (9) T_{if}^D represents the rearrangement induced by the distortion in the final channel. We should like to mention at this point that it is desirable to represent the exact scattering state as accurately as practically possible by the distorted wave since a perturbation treatment of the residual interaction is then more likely to be valid. In other words, it is very attractive to define distorted waves in the final channel which are asymptotically nonorthogonal to the initial state in such a way that the distortion part T_{if}^D is nonvanishing. Note that this approach is uncommon in previous applications of distorted-wave theory. The example discussed in Sec. III A is to our knowledge the first practical example of distorted waves which accommodate the rearrangement in question.

Equations (15) and (16) contain a remarkable extension of the well-known post-prior equivalence of the first Born approximation: If the distortion in the final channel is chosen so that it does not connect to the initial state ($T_{if}^D = 0$) the following equality holds on the energy shell,

$$\langle \chi_f^- | W_f^{\dagger} | \Phi_i \rangle = \langle \chi_f^- | V_i | \Phi_i \rangle \ . \tag{17}$$

An application of Eq. (17) will be discussed in Sec. III B.

B. Impact-parameter formulation

In the time-dependent formulation[13] an exact scattering state is sought as a solution to the time-dependent Schrödinger equation

$$\left[i \frac{\partial}{\partial t} \bigg|_r - H(t) \right] |\psi_i^{\pm}(t)\rangle = 0 \tag{18}$$

subject to the boundary condition

$$|\psi^+(t)\rangle \to |\phi_i(t)\rangle \quad \text{for } t \to -\infty \ ,$$

where $|\phi_i(t)\rangle$ is an eigenstate of the time-independent initial channel Hamiltonian H_i. [Here and throughout this section it is understood that all states are appropriately Galilei-transformed to the inertial frame implied by Eq. (18).] The exact transition amplitude is given by

$$a_f = \lim_{t \to \infty} \langle \phi_f(t) | \psi_i^+(t) \rangle \ , \tag{19}$$

where $|\phi_f(t)\rangle$ is an eigenstate of the time-independent Hamiltonian H_f belonging to the final channel. In place of Eq. (19) the exact amplitude may also be calculated from a t-matrix expression obtained by integration of the time derivative of the matrix element, i.e.,

$$a_f = -i \int_{-\infty}^{\infty} dt \langle \phi_f(t) | H - H_f | \psi_i^+(t) \rangle \tag{20}$$

since the surface term $\langle \phi_f(t) | \psi_i^+(t) \rangle$ vanishes in the limit $t \to -\infty$ for bound initial and final states.

Distorted waves are defined as solutions to the time-dependent Schrödinger equation corresponding to distorted channel Hamiltonians. In the final channel we have

$$\left[i \frac{\partial}{\partial t} \bigg|_r - H_f - U_f(t) \right] |\chi_f^-(t)\rangle = 0 \tag{21}$$

subject to the boundary condition

$$|\chi_f^-(t)\rangle \to |\phi_f(t)\rangle \quad \text{for } t \to \infty \ .$$

Then the t-matrix expression for the transition amplitude becomes

$$a_f = -i \int_{-\infty}^{\infty} dt \langle \chi_f^-(t) | W_f^\dagger | \psi_i^+(t) \rangle + a_f^D \ , \tag{22}$$

where $W_f = H - H_f - U_f$ and the surface term a_f^D is given by

$$a_f^D = \lim_{t \to -\infty} \langle \chi_f^-(t) | \phi_i(t) \rangle \tag{23}$$

and clearly represents the transition amplitude due to distortion in the final channel.

Applying the t-matrix expression to the transition amplitude in Eq. (23) and noting that $\langle \chi_f^-(t) | \phi(t) \rangle$ vanishes in the limit $t \to +\infty$, we find

$$a_f^D = -i \int_{-\infty}^{\infty} dt \langle \chi_f^-(t) | V_i - W_f^\dagger | \phi_i(t) \rangle \ . \tag{24}$$

The form (22) is accordingly entirely equivalent to the quantal expression (14). In either case the total transition amplitude appears as a sum of two terms, one due to the distortion and the other due to the residual part of the channel interaction.

C. Distorted-wave series

Since the method of integral equations and series expansions generally involves off-energy-shell extensions and since our treatment of the distortion part of the T matrix is valid only on the energy shell, it is essential to restrict series expansions to the residual part of the T matrix. We therefore write the post form of the T matrix as

$$T_{if} = T_{if}^D + \langle \Phi_f | T^R | \Phi_i \rangle \ , \tag{25}$$

where, according to Eqs. (5), (11), and (14) the operator T^R is defined as

$$T^R = (\omega_f^-)^\dagger W_f^\dagger \Omega_i^+ \ . \tag{26}$$

A standard iteration of the exact Møller operator Ω_i^+ in terms of the corresponding distorted-wave operator ω_i^+ then generates the following integral equation as first noted by Greider and Dodd:[14]

$$T^R = (\omega_f^-)^\dagger W_f^\dagger \omega_i^+ + T^R K \ , \tag{27}$$

where the integral kernel K is given by

$$K = G_i^+ W_i \omega_i^+ \tag{28}$$

and $G_i^+ = (E - H_i + i\eta)^{-1}$ is the Green's operator in the initial channel. It is interesting to note that the form of K is independent of the choice of distortion in the final channel.

A general assessment of the convergence properties of Eq. (27) is not feasible at present. However, it is crucial that the kernel (28) connects all particles of the problem since the Neumann series solution to Eq. (27) otherwise will contain subseries of terms that correspond to a situation where one of the three particles propagates freely [Fig. 1(a)]. As shown by Aaron *et al.*[15] such subseries are usually divergent. We shall see in the next section that a class of modern theories for electron capture uses a truly connected kernel. In the present case the statement that disconnected diagrams are absent is more restrictive than in the general three-body scattering case[14] since we have omitted one of the three interactions, the internuclear potential, from the onset. The kernel can contain only connected diagrams involving electron-nucleus interactions [Fig. 1(b)] whereas a general three-body diagram may be connected by an internuclear interaction but might be disconnected otherwise [Fig. 1(c)].

In the absence of disconnected diagrams the source term in Eq. (27),

$$T_{if}^{R1} = \langle \chi_f^- | W_f^\dagger | \chi_i^+ \rangle \ , \tag{29}$$

represents a consistent first-order theory and a single iteration of Eq. (27),

$$T_{if}^{R2} = \langle \chi_f^- | W_f^\dagger \omega_i^+ G_i^+ W_i | \chi_i^+ \rangle \ , \tag{30}$$

is a measure of the error introduced by the first-order approximation. Expanding the Green's operator in a complete set of eigenstates for the target Hamiltonian such that

$$\omega_i^+ G_i^+ = \sum_n |\chi_n^+\rangle (E - E_n + i\eta)^{-1} \langle \Phi_n | \tag{31}$$

it is seen that Eq. (30) involves off-shell generalizations of the first-order approximation (29).

III. EXAMPLES

The undistorted channel states and the exact scattering states represent two extremes. The initial or final channel

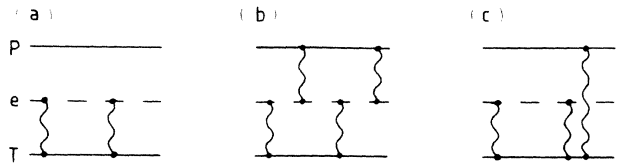

FIG. 1. (a) Example for a disconnected diagram; (b) connected diagram involving only electron-nucleus interactions; (c) diagram connected by an internuclear interaction while disconnected when only electron-nucleus interactions are taken into account.

state is generally available as a product of a free wave, which describes the motion of the free nucleus relative to the center of mass of the composite system, and a bound state which represents the internal structure of the initial or final state. The multichannel scattering states are, on the other hand, not available in exact form. The distorted waves may represent a suitable compromise. They may account for an important part of the channel interaction and nevertheless be computable in practice. The essential point is that the residual part of the channel interaction is reduced sufficiently to allow a perturbation treatment.

The application[6,7] of the SPB states in distorted-wave theory is discussed in the first example. These states are sophisticated enough to account for a significant part of the capture amplitude. The price to pay for this is that the matrix elements of the residual interaction between distorted waves are very difficult to evaluate. The simpler CDW's are discussed in the second example. The matrix elements are then much easier to evaluate. The price for this is that a first-order treatment is not necessarily sufficient.

A. Strong-potential distorted waves

The approximate scattering state applied in the post form of the SPB approximation[16] is given by

$$|\chi_i^{+(\mathrm{SPB})}\rangle=\omega_P^+|\Phi_i\rangle=(1+G_P^+V_P)|\Phi_i\rangle\ , \tag{32}$$

where $G_P^+=[E-(H_0+V_P)+i\eta]^{-1}$ is the projectile Green's operator. The underlying physical picture in Eq. (32) is as follows. The electronic part of Φ_i is a bound state, localized in a narrow region around the target nucleus. This bound state may be viewed as a wave packet incident on the projectile nucleus. The electronic part of the SPB state in Eq. (32) is essentially the corresponding packet of elastically scattered waves. The only difference is that while each momentum component of a wave packet in potential scattering theory scatters under conservation of its own kinetic energy, the SPB wave in Eq. (32) conserves the total energy of the initial state in such a way that individual momentum components in (32) generally scatter off the energy shell.

Since off-energy-shell potential scattering is not more difficult than on-shell scattering, it is clear that the SPB wave is computable in practice. In fact, the SPB wave is optimal within the single channel limitation of potential scattering since it accounts exactly for the scattering of the target-centered wave packet in the projectile field.

The SPB wave in Eq. (32) clearly represents a particularly important distortion of the initial state in the strong projectile limit, $Z_P\gg Z_T$. A corresponding strong target distortion of the final state is represented by

$$|\chi_f^{-(\mathrm{SPB})}\rangle=\omega_T^-|\Phi_f\rangle=(1+G_T^-V_T)|\Phi_f\rangle\ , \tag{33}$$

where $G_T^-=[E-(H_0+V_T)-i\eta]^{-1}$ is the target Green's operator.

The SPB states (32) and (33) are generated by the distortions

$$U_i=V_P-V_TG_0^+V_P \tag{34}$$

and

$$U_f=V_T-V_PG_0^-V_T\ , \tag{35}$$

where $G_0^\pm=(E-H_0\pm i\eta)^{-1}$ is the free Green's operator. The residual interactions are accordingly equivalent to the double-scattering operator,

$$W_i=W_f^\dagger=W=V_TG_0^+V_P\ . \tag{36}$$

The proof of Eqs. (34) and (35) was implicitly given in Ref. 7. In Appendix A we demonstrate explicitly that the distortions U in Eqs. (34) and (35) generate the SPB waves of Eqs. (32) and (33).

1. *The surface term*

Using Eqs. (33) and (36) it is readily shown that the surface term T_{if}^D in the post form of the distorted-wave T matrix given by Eq. (14) may be expressed as[7]

$$T_{if}^D=\langle\phi_f|V_P|\phi_i\rangle=T_{if}^{\mathrm{B1}} \tag{37}$$

which is the first Born (Brinkman-Kramers) approximation for the electron capture T matrix. Similarly it may be shown that the surface term (24) of the impact-parameter formulation also is identical to the first Born capture amplitude.

While the first Born approximation under suitable conditions is a valuable approximation for excitation and ionization processes it is now generally appreciated[16] that the B1 approximation for capture is hardly justified. It is therefore very satisfactory that the SPB distorted waves already contain this term in zeroth order in such a way that only the multiple scattering part of the T matrix has to be treated by perturbation or iteration.

2. *The distorted-wave Born series*

Using the distorted-wave Møller operators belonging to the SPB waves as defined in Eqs. (32) and (33) and the explicit form (36) of the corresponding residual interaction, the integral equation (27) becomes

$$T^R=(1+V_TG_T^+)V_TG_0^+V_P(1+V_PG_P^+)+T^RK\ , \tag{38}$$

where

$$K=G_T^+V_TG_P^+V_P\ . \tag{39}$$

Adding the surface term (37) to the matrix element of the source term on the right-hand side (rhs) of the integral equation (38) we obtain the symmetric first DWB approximation

$$T_{if}^{\mathrm{DWB}}=T_{if}^{\mathrm{B1}}+\langle\chi_f^{-(\mathrm{SPB})}|V_TG_0^+V_P|\chi^{+(\mathrm{SPB})}\rangle\ . \tag{40}$$

As noted in Ref. 7 the DWB contains all terms of single switch character in the ordinary Born series. This is most easily seen from Eq. (39) where an expansion of the G_T^+ and G_P^+ operators in the first-order term gives rise to a series of terms all of which are characterized by the fact that the sequence of operators begins with a sequence of V_P operators on the right and changes only once to end with a sequence of V_T operators on the left. The kernel K in Eq. (39) is, on the other hand, a double switch generator. This implies that the first iteration of Eq. (38) supplies all terms of triple switch character and that subsequent iterations are characterized by their odd number of

switches. The number of switches may be identified as a measure of the degree of connectedness of terms in the T matrix. The terms of the DWB series, generated by iteration of Eq. (38), are therefore progressively more and more connected. This is expected to be a key feature of a rapidly converging series since each switch involves an appreciable amount of momentum transfer to counterbalance the relative translation of the two nuclei.

Alston[17] has noted that the DWB approximation (40) also may be expressed as

$$T_{if}^{\mathrm{DWB}} = T_{if}^{\mathrm{B1}} + \langle \Phi_f \mid T_T G_0^+ T_P \mid \Phi_i \rangle \tag{41a}$$

$$= T_{if}^{\mathrm{B1}} + \langle \Phi_f \mid V_T G_T^+ T_P \mid \Phi_i \rangle \ , \tag{41b}$$

where T_T and T_P denote the transition operators $V_T + V_T G_T^+ V_T$ and $V_P + V_P G_P^+ V_P$, respectively.

Equation (41a) is particularly interesting because it shows that the DWB approximation is equivalent to the Faddeev-Watson approximation[17] with a vanishing internuclear potential. The physical intuition implemented in the distorted-wave formulation therefore may be used to improve the general understanding of the underlying physics of the Faddeev expansion. We employ the DWB approximation in the following to clarify the conceptual foundation of the strong-potential Born approximation as applied to asymmetric collision systems. In particular, we resolve the divergence problem recently identified by Dewangan and Eichler.[18]

3. *The strong-potential Born limit*

The familiar SPB expansion of the T operator reorders the ordinary Born series according to powers of the weaker potential. The strong target SPB expansion reads

$$T = V_P + V_T G_T^+ V_P + V_T G_T^+ V_P G_T^+ V_P + \cdots \ . \tag{42}$$

The first two terms on the rhs of Eq. (42) are both of first order in the weak potential V_P and these are commonly known as the SPB approximation,

$$T_{if}^{\mathrm{SPB}} = \langle \Phi_f \mid (1 + V_T G_T^+) V_P \mid \Phi_i \rangle \ . \tag{43}$$

Equation (42) is also obtained by iteration of the integral equation (27) of the distorted-wave formulation of Sec. II C by ignoring the distortion in the initial channel but retaining the SPB distortion in the final channel, i.e.,

$$\omega_i^+ = 1, \quad \omega_f^- = \omega_T^- \ , \tag{44}$$

such that the integral kernel becomes $K = G_T^+ V_P$. Since

$$K = G_T^+ V_P = G_0^+ V_P + G_T^+ V_T G_0^+ V_P = K_0 + K_1 \ , \tag{45}$$

it is seen that the kernel K contains the disconnected part $K_0 = G_0^+ V_P$. This implies that the SPB expansion in Eq. (42) may contain divergent subseries[14] of disconnected terms. Formally, however, we may resum these critical subseries. As an example, the subseries of terms that results from the K_0 part only may be summed to give

$$V_T G_T^+ V_P \sum_{n=1}^{\infty} (G_0^+ V_P)^n = V_T G_T^+ V_P G_P^+ V_P \ . \tag{46}$$

This equation provides the sequence of single switch terms which are of second or higher order in the weak potential V_P. The contribution may therefore be expected to be small in the weak-potential limit, provided that the operator series converges. As shown by Aaron *et al.*[15] this is, however, not generally the case. The SPB expansion is therefore not quite justified. This does not necessarily mean that the first SPB approximation to the T-matrix element is wrong. In fact, in the following we shall present two alternative derivations which lead to the SPB approximation in a more satisfactory way. First, we identify the SPB approximation as the source term of an integral equation with a connected kernel. Secondly, we consider the well-behaved DWB approximation in the limit of asymmetric collisions and derive a slightly modified version of the SPB approximation.

To show that the SPB approximation belongs to an integral equation with a connected kernel we start from the prior instead of the post form of the exact T operator. Then, Eq. (27) is replaced by

$$T^R = (\omega_f^-)^\dagger W_i \omega_i^+ + K T^R \tag{47}$$

with

$$K = (\omega_f^-)^\dagger W_f^\dagger G_f^+ \ . \tag{48}$$

In the prior form there is generally a contribution to the T-matrix element from the distortion in the initial channel similar to the distortion part given by Eqs. (15) and (16). In the specific case of a strong target potential [Eq. (44)] there is no distortion in the initial channel and we obtain

$$T^{R1} = (\omega_T^-)^\dagger V_P = V_P + V_T G_T^+ V_P = T^{\mathrm{SPB}} \tag{49}$$

for the source term in Eq. (47) and

$$K = V_T G_T^+ V_P G_P^+ \tag{50}$$

for the integral kernel. Since this kernel is a double switch generator it may be expected that the pertaining series solution has satisfactory convergence properties. The price to pay for the absence of disconnected terms is that the series solution is no longer ordered according to powers of the weaker potential, neither is it completely ordered according to the number of switches. The second-order term is, for example, given by

$$T^{R2} = V_T G_T^+ V_P G_P^+ V_P + V_T G_T^+ V_P G_P^+ V_T G_T^+ V_P \ , \tag{51}$$

i.e., a sum of single and triple switch terms. Note that the first term on the rhs of Eq. (51) is identical to the rhs of Eq. (46). As we shall argue in the following it is important to include the part of this term that corresponds to intermediate propagation in the initial bound state of the electron, i.e., the contribution from intermediate elastic scattering.

The distorted-wave expansion of Eq. (38) is, in contrast to the strong-potential expansion of Eq. (42), a consistent series expansion with a connected integral kernel. Noting that the troublesome series in Eq. (46) precisely provides those terms of the first DWB approximation which were left out in the SPB approximation it is tempting to seek a justification of the SPB approximation within the more general DWB approximation. This involves a consistent

approach to the asymmetric limit, $Z_P \ll Z_T$. Comparing Eq. (43) with Eq. (41b) it is seen that the SPB approximation is obtained from the DWB approximation if the operator T_P is replaced by V_P. This is the first Born approximation for the T operator of the weak field. To discuss the validity of this approximation it is useful to expand the DWB expression Eq. (41b) in a complete set of target channel states, $|\Phi_n^T(\mathbf{K})\rangle$, where, for later convenience, the wave vector $\mathbf{K}$ of relative nuclear motion is given explicitly. Specifying, by superscript on the channel state, the nucleus to which the electron is attached, we obtain

$$T_{if}^{\mathrm{DWB}} = T_{if}^{\mathrm{B1}} + \sum_n \int d\mathbf{K} \frac{\langle \Phi_f^P(\mathbf{K}_f) | V_T | \Phi_n^T(\mathbf{K})\rangle \langle \Phi_n^T(\mathbf{K}) | T_P | \Phi_i^T(\mathbf{K}_i)\rangle}{E - E_n(K) + i\eta} . \tag{52}$$

It is accordingly seen that the SPB is a valid approximation to the DWB if and only if the first Born approximation for scattering into arbitrary target states is valid in magnitude as well as phase.

The Born approximation is generally accepted to be valid for target excitation and ionization so long as $Z_P \ll Z_T$. The situation is different for elastic scattering, $n = i$. The Born approximation for elastic scattering is often considered to be a high-velocity approximation, valid for $v \gg Z_P$, i.e., in the region where the target SPB normally is considered to apply, but this is only true so far as the magnitude of the T matrix is concerned. The phase of the T matrix is in fact poorly represented at small momentum transfer for the type of potentials that are of interest in atomic physics.[19] The SPB approximation is accordingly only a valid approximation to the DWB approximation in the limit of asymmetric collisions $Z_P \ll Z_T$ if it is modified properly to account correctly for propagation in the initial state $n = i$.

A correct treatment of the limit $Z_P \ll Z_T$ of the DWB approximation solves the problem spotted by Dewangan and Eichler[18] concerning the singular contribution from intermediate scattering in the initial electron state in the ordinary SPB approximation for bare Coulomb potentials. These authors noted that

$$\langle \Phi_n^T(\mathbf{K}) | V_P | \Phi_i^T(\mathbf{K})\rangle \propto |\mathbf{K} - \mathbf{K}_i|^{-2} \tag{53}$$

for $n = i$ and that the divergence at small momentum transfer of this term in the SPB form of Eq. (52) coalesces with the corresponding initial ground-state pole in the Green's function to produce a nonintegrable singularity.

In the following we show that a DWB treatment yields a finite contribution from intermediate propagation in the initial state. First we note that

$$T_P(E) = V_P + V_P(E - H_P + i\eta)^{-1} V_P \tag{54}$$

is a three-body operator since the Hamiltonian H_P contains the kinetic energy operator corresponding to the free motion of the target nucleus with respect to the center of mass of the projectile-electron system. Considering the relevant matrix element $T_P(E)$ in Eq. (52),

$$I = \langle \Phi_i^T(\mathbf{K}) | T_P(E) | \Phi_i^T(\mathbf{K}_i)\rangle \tag{55}$$

it is, however, not difficult to perform the integral over this coordinate to obtain

$$I = \int d^3p\, \tilde{\phi}_i(\mathbf{p}+\mathbf{v}) \tilde{\phi}_i(\mathbf{p}+\mathbf{v}+\mathbf{K}_i-\mathbf{K}) t_P(\mathbf{p}, \mathbf{p}+\mathbf{K}_i-\mathbf{K}; \epsilon) , \tag{56}$$

where $\tilde{\phi}$ is the initial electron state in momentum representation and t_P is the electron-projectile two-body T matrix in momentum representation at the energy

$$\epsilon = \tfrac{1}{2}p^2 + \epsilon_i - \tfrac{1}{2}(\mathbf{v}+\mathbf{p})^2 . \tag{57}$$

Here, ϵ_i is the binding energy of the initial electron state and $\mathbf{v}$ is the impact velocity. Since ϵ certainly is smaller than $\frac{1}{2}p^2$ it is clear that the two-body scattering in Eq. (56) takes place off the energy shell. The t_P matrix in Eq. (56) is accordingly well defined[20] also for the unscreened Coulomb case.

We may evaluate Eq. (56) at high velocities $v \gg Z_T$ in the near-energy-shell approximation[20] to obtain

$$I = -\frac{1}{2\pi^2} \frac{Z_P}{|\mathbf{K}-\mathbf{K}_i|^2} (|\mathbf{K}-\mathbf{K}_i|^2/8\epsilon)^{i\nu_P} \exp[2i \arg\Gamma(1+i\nu_P)]$$
$$\times \int d^3p\, \tilde{\phi}_i(\mathbf{p}+\mathbf{v}) \tilde{\phi}_i(\mathbf{p}+\mathbf{v}+\mathbf{K}-\mathbf{K}_i) g(p) g(|\mathbf{p}+\mathbf{K}_i-\mathbf{K}|) , \tag{58}$$

where $\nu_p = Z_P/v$ and the off-energy-shell factor $g(p)$ is given by

$$g(p) = \left[\frac{\epsilon - \frac{1}{2}p^2}{\epsilon}\right]^{-i\nu_P} \Gamma(1 - i\nu_P) \exp(-\nu_P \pi/2) , \tag{59}$$

The integral in Eq. (58) is seen to be a smooth function of $\mathbf{K}$ in the vicinity of $\mathbf{K}_i$. Upon inserting Eq. (58) into Eq. (52) the critical contribution from forward angles $\mathbf{K} \sim \mathbf{K}_i$ in the integral over $\mathbf{K}$ may therefore be estimated in a peaking approximation to be proportional to the integral

$$\int d^3\mathbf{K} (K_i^2 - K^2 + i\eta)^{-1} (|\mathbf{K}-\mathbf{K}_i|)^{-2+2i\nu_P} . \tag{60}$$

If the Coulomb phase factor $|\mathbf{K}-\mathbf{K}_i|^{2i\nu_P}$ is neglected, the integral is logarithmically singular as noted by Dewangan and Eichler.[18] It is finite when the Coulomb phase factor is properly retained.[30]

Let us emphasize that the problem with the intermediate state propagation is particularly dramatic but certainly

not peculiar to the Coulomb case since the Born approximation is generally invalid in the calculation of the phase of the elastic scattering amplitude for realistically screened atomic potentials as already mentioned above. Also it should be noted that a contribution from the ground-state pole is physically reasonable as it is certainly present in an exact representation of the capture T matrix. In other words, the pole contribution is not spurious. It must be evaluated, however, with sufficient care as indicated above. Whether the modified contribution from the initial state pole is actually negligible as implied in previous evaluations[21,22] remains to be tested.

The impact-parameter version of the ordinary SPB approximation is naturally also divergent[18] due to the improper treatment of the intermediate propagation in the initial electron state. It is easily seen that the singularity may be removed by including the elastic scattering in the initial state similar to the present treatment in the full quantal picture. Alternatively, it may be sufficient to include, for example, the eikonal phase of the elastic scattering in the weak field.

A comparison with the standard treatment of secular terms in the impact-parameter method is instructive. In the close-coupling picture, elastic propagation in the various channels is determined by the diagonal terms of the coupling matrix. It is well known[6,13] that it is essential to remove these so-called secular terms of the coupling matrix by a phase transformation in order to improve the convergence of the time integration. In fact, the time integration does not converge in the case of Coulomb interactions unless this transformation is employed.

B. Continuum distorted waves

The CDW functions[1] have a simple form in coordinate space in terms of sets of Jacobi coordinates $(\mathbf{r}_T,\mathbf{R}_T)$ or $(\mathbf{r}_P,\mathbf{R}_P)$. Here $\mathbf{r}_T$ is the electron position vector with respect to the target while $\mathbf{R}_T$ determines the position of the projectile with respect to the center of mass of the target atom. The set $(\mathbf{r}_P,\mathbf{R}_P)$ is defined similarly. The coordinate representation of the CDW functions is then

$$\chi_i^{+(\mathrm{CDW})}(\mathbf{r}_T,\mathbf{R}_T)=N(\nu_P)\,{}_1F_1(i\nu_P,1,i(vr_P+\mathbf{v}\cdot\mathbf{r}_P))\times\Phi_i(\mathbf{r}_T,\mathbf{R}_T) \tag{61a}$$

and

$$\chi_f^{-(\mathrm{CDW})}(\mathbf{r}_P,\mathbf{R}_P)=N^*(\nu_T)\,{}_1F_1(-i\nu_T,1,-i(vr_T+\mathbf{v}\cdot\mathbf{r}_T))\times\Phi_f(\mathbf{r}_P,\mathbf{R}_P)\ , \tag{61b}$$

where $N(\nu_{P,T})$ denotes the normalization factor for a Coulomb wave and $\nu_{P,T}=Z_{P,T}/v$.

The CDW waves in the impact-parameter version are also given by Eqs. (61), but with a prescribed internuclear trajectory, $\mathbf{R}_T\cong\mathbf{R}_P\cong\mathbf{R}(t)$. The CDW partitioning of the channel interaction is only available in implicit form. Considering the final channel the residual interaction is given by

$$W_f\chi_f^{-(\mathrm{CDW})}(\mathbf{r}_P,\mathbf{R}_P)=-N^*(\nu_T)(2\pi)^{-3/2}\exp(i\mathbf{K}_f\cdot\mathbf{R}_P)[\nabla_{\mathbf{r}_T}\,{}_1F_1(-i\nu_T,1,-i(vr_T+\mathbf{v}\cdot\mathbf{r}_T))]\cdot[\nabla_{\mathbf{r}_P}\phi_f(\mathbf{r}_P)]\ . \tag{62}$$

The residual interaction in the initial channel is given by a similar expression.

1. The surface term

It is clear from Eq. (23) that the surface term of the continuum distorted-wave amplitude for electron capture vanishes in the impact-parameter formulation because $\chi_{i,f}^{\pm(\mathrm{CDW})}(\mathbf{r},t)$ remains well localized around the parent nucleus such that the overlap vanishes asymptotically. This suggests that the distortion part of the quantal T matrix also must vanish. That this is actually the case is demonstrated explicitly in Appendix B. Parenthetically we note that the surface term may be finite for direct excitation.

An immediate consequence of the asymptotic orthogonality of the CDW waves is the strict equivalence of the peaked impulse approximation (PIA) and the so-called method I proposed by Cheshire.[1] It has been known for a long time that the two approximations give identical numerical results for hydrogenic systems.[2] The identity (17) provides a simple and general proof. Applied to the CDW case the left- and right-hand sides of Eq. (17) may be identified with the prior form of the T matrix in Cheshire's method I and in the PIA, respectively.

2. The continuum distorted-wave series

The CDW series expansion is obtained from the general formulation of Sec. II C if both channels are considered to be distorted in the CDW sense. It is seen that the pertaining integral kernel, as given by Eq. (28), is free of disconnected terms. This property follows directly from the fact that a single residual interaction W_i [Eq. (50)] affects all internal coordinates simultaneously. The CDW series is obtained by the usual iteration procedure from the integral equation (27) in T^R which in the CDW case represents the complete T operator since the surface term vanishes. The fact that the kernel of the integral equation connects all degrees of freedom of the system suggests that the CDW Born series has acceptable convergence properties. But it does not guarantee that the series is well represented by its first term. The latter requires in addition that the distorted waves are good approximations to the exact scattering states. The CDW waves are obtainable from the SPB waves if off-energy-shell effects are ignored as in the impulse approximation and if a peaking approximation is applied to eliminate the integration over the electron momentum distribution in the considered channel.[16] This would suggest that the CDW waves are reasonable high-velocity approximations and that the first-order approximation for the T-matrix element

$$T_{if}^{\mathrm{CDW1}}=\langle\chi_f^{-(\mathrm{CDW})}\,|\,W_f^{\dagger}\,|\,\chi_i^{+(\mathrm{CDW})}\rangle\ , \tag{63}$$

where $W_f\,|\,\chi_f^{-(\mathrm{CDW})}\rangle$ is given by Eq. (62), is valid at sufficiently high velocities. As we shall discuss in detail in the following section, however, this is not correct.

Higher-order terms of the CDW series must be included even at high velocities. Including terms to second order in the CDW Born series one obtains

$$T_{if}^{\mathrm{CDW2}} = T_{if}^{\mathrm{CDW1}} + \sum_n \langle \chi_f^{-(\mathrm{CDW})} \mid W_f^\dagger \mid \chi_n^{+(\mathrm{CDW})} \rangle \times (E - E_n + i\eta)^{-1} \times \langle \phi_n \mid W_i \mid \chi_i^{+(\mathrm{CDW})} \rangle , \quad (64)$$

where the summation extends over a complete set of initial channel states.

3. *The CDW in the Thomas peak region*

It is widely accepted that capture at asymptotically high velocities is intimately connected with the double-scattering mechanism proposed by Thomas.[23] In this classical process electron capture is described as a sequence of two binary collisions: a quasifree electron is first scattered off the projectile through an angle of 60° with respect to the projectile velocity **v** and then scattered through 60° off the target in such a way as to leave the electron with almost zero velocity in the rest frame of the projectile. Quantum mechanically the Thomas process is represented by the B2 (second Born) term, or more precisely, by that part of the second Born term that corresponds to propagation in energy-conserving intermediate states.[24] A unique signature of the double scattering contribution is the Thomas peak in the differential capture cross section $\sigma(\theta)$ at a projectile scattering angle $\theta_T = \sqrt{3} m_e / M_P$ (M_P is projectile mass, m_e is electron mass). Rivarola and Miraglia[4] have shown that the CDW1 approximation for ground-state to ground-state transfer displays a narrow dip precisely at the Thomas angle. McGuire *et al.*[24] found a similar dip in the differential B2 cross section at the Thomas angle if only off-the-energy-shell intermediate propagation was included. This indicates that the CDW1 approximation lacks a contribution that corresponds to classical Thomas scattering. In an approximate CDW2 calculation for $1s \rightarrow 1s$ capture Crothers and McCann[10] have demonstrated that the dip at the Thomas angle disappears when the second-order term in (64) is included. Very recently, Crothers[11] has achieved a major breakthrough by proving the equivalence of the CDW2 and second Born amplitudes at asymptotically high velocities for transitions between hydrogenic states $1s \rightarrow nlm$. In the following we examine the behavior of the second-order contribution to the CDW t matrix from a somewhat different point of view. We investigate the second part of the CDW amplitude [Eq. (64)] for arbitrary initial and final states in the limited kinematic region that corresponds to the classical Thomas scattering and show that the classical Thomas contribution indeed is contained in this term. Since the large momentum transfer between the two nuclei in the classical Thomas mechanism is mediated by an electron which, independent of the internal momentum distribution of the initial and final states, propagates with high momentum between the two collisions we therefore approximate the second-order part of the CDW2 amplitude as

$$\langle \chi_f^{-(\mathrm{CDW})} \mid W_f^\dagger G_0^+ W_i \mid \chi_i^{+(\mathrm{CDW})} \rangle = \int d^3\mathbf{p} \int d^3\mathbf{P} \langle \chi_f^{-(\mathrm{CDW})} \mid W_f^\dagger \mid \Phi_{\mathbf{p},\mathbf{P}} \rangle (E - E_{\mathbf{p},\mathbf{P}} + i\eta)^{-1} \times \langle \Phi_{\mathbf{p},\mathbf{P}} \mid W_i \mid \chi_i^{+(\mathrm{CDW})} \rangle , \quad (65)$$

where $\mid \Phi_{\mathbf{p},\mathbf{P}} \rangle$ is a free-particle state of energy $E_{\mathbf{p},\mathbf{P}}$. Referring explicitly to the target set of Jacobi coordinates the complete set of intermediate states is given by

$$\langle \mathbf{r}_T, \mathbf{R}_T \mid \Phi_{\mathbf{p},\mathbf{P}} \rangle = (2\pi)^{-3} \exp[i(\mathbf{p}\cdot\mathbf{r}_T + \mathbf{P}\cdot\mathbf{R}_T)] . \quad (66)$$

We have evaluated the second-order term in Eq. (65) to first order in v_P and v_T where $v_P = Z_P/v$ and $v_T = Z_T/v$. The evaluation proceeds in close analogy to that of the second Born term.[25] Details are given in Appendix C. The result is

$$\langle \chi_f^{-(\mathrm{CDW})} \mid W_f^\dagger G_0^+ W_i \mid \chi_i^{+(\mathrm{CDW})} \rangle \cong (2\pi)^{-3} \int d^3\mathbf{k} \int d^3\mathbf{q}\, \tilde{\phi}_f^*(\mathbf{k}) \tilde{V}_f(\mathbf{q}+\mathbf{J}) N_f \times [\epsilon_i - \tfrac{1}{2}K^2 - \tfrac{1}{2}(\mathbf{q}+\mathbf{k})^2 + \mathbf{v}\cdot(\mathbf{k}-\mathbf{K}) + \mathbf{K}\cdot(\mathbf{q}+\mathbf{k}) + i\eta]^{-1} N_i \tilde{V}_P(\mathbf{k}-\mathbf{K}) \tilde{\phi}_i(\mathbf{q}) , \quad (67)$$

where ϵ_i is the internal binding energy of the initial state, **K** is the momentum transfer, $\mathbf{K} \cong \mathbf{K}_f - \mathbf{K}_i$, and $-\mathbf{J} = \mathbf{K} + \mathbf{v}$.

This agrees with the double-scattering term[25] in the B2 approximation except for presence of the vertex renormalization factors $N_{i,f}$ in the integral with

$$N_i = \frac{\mathbf{q}\cdot(\mathbf{k}-\mathbf{K})}{(v + \mid \mathbf{k}-\mathbf{K}-\mathbf{v} \mid)(v - \mid \mathbf{k}-\mathbf{K}-\mathbf{v} \mid + i\epsilon)} \quad (68a)$$

and

$$N_f = \frac{\mathbf{k}\cdot(\mathbf{q}+\mathbf{J})}{(v + \mid \mathbf{q}+\mathbf{J}+\mathbf{v} \mid)(v - \mid \mathbf{q}+\mathbf{J}+\mathbf{v} \mid - i\epsilon)} . \quad (68b)$$

These factors contain poles representing elastic scattering at the "active" nucleus of a free electron with velocity $(\pm\mathbf{v})$ and zero momentum spread. These poles will play an important role when the dominant capture mechanism is a sequence of two elastic binary collisions and when the internal momentum distribution of the initial and final state is negligible. This is precisely the situation corresponding to "classical" Thomas scattering at asymptotically high velocities.

We will now investigate the behavior of the renormalization factors in (68) near the Thomas angle. At high collision velocities the internal momenta **q** and **k** are small compared to **v**. Near the pole of the free-particle propagator in (67) at $K_{\parallel} \cong -\frac{1}{2}v$ and $K_{\perp} = (\sqrt{3}/2)v$, the denominators in (68) can be expanded to first order in **k** and **q** as

$$N_i \cong \mathbf{q}\cdot(\mathbf{K}-\mathbf{k})/\mathbf{J}\cdot\mathbf{k} \quad (69a)$$

and

$$N_f \cong \mathbf{k}\cdot(\mathbf{J}+\mathbf{q})/\mathbf{k}\cdot\mathbf{q} \tag{69b}$$

to show that the product of these two factors approaches unity in this region. The matrix element

$$\langle \chi_f^{-(\mathrm{CDW})} \mid W_f^{\dagger} G_0^{+} W_i \mid \chi_i^{+(\mathrm{CDW})} \rangle$$

therefore becomes equal to the double-scattering term of the B2 amplitude at the Thomas peak. In other words, the term left out in the CDW1 approximation contains that portion of the on-shell Thomas double-scattering term in the Born series for which the internal momentum distribution is negligible. In this sense, the CDW1 approximation is incomplete with respect to the B2 approximation. This result is in complete accord with previous findings by Crothers.[10,11] A correct description of the double-scattering term therefore requires the second-order CDW approximation.

IV. CONCLUSIONS

Two questions generally arise in connection with distorted-wave theories for three-body rearrangement scattering. The first concerns the possible rearrangement induced by the distortion itself. The second question concerns the convergence properties of the resulting distorted-wave Born series. In this connection we may identify two extreme types of distortions. We refer to them as substantial and marginal, respectively.

A substantial distortion induces a significant physical part of the transition amplitude for rearrangement on its own such that the remaining part of the T matrix is better suited for a perturbation treatment and it provides a perturbation expansion in the residual interaction with an integral kernel which connects the different arrangement channels. The other extreme is the marginal distortion which does not satisfy any of these conditions.

We have shown in the present work that the DWB theory with SPB distortion in both channels satisfies all requirements for a substantial distortion and is therefore expected to have good convergence properties. While from a mathematical point of view a connected kernel is a necessary (but not sufficient) condition for the perturbation series to converge it is physically very plausible that the switches between target and projectile interactions, as generated by the DWB integral kernel, provide a sensible order parameter for a perturbation series at high energies.

The situation is less promising if the SPB distortion is applied only in one of the two channels. The SPB series ordered in powers of the weak potential does not possess a connected kernel but the distortion induces rearrangement. A different series with the full SPB approximation as first-order term but with the same integral kernel as in the complete DWB series is an example of a perturbation series with a connected kernel. The price to pay is that the series is no longer ordered in powers of the weak potential and, in addition, that the distortion itself does not contribute to the transition amplitude. In either case it is important to reorder terms to obtain certain satisfactory features of a substantial distortion. A study of these two different limiting cases of the full DWB theory provides also a method to remove the nonintegrable singularity in the ordinary SPB approximation recently discussed by Eichler and Dewangan by defining a consistent limit of the DWB approximation in the asymmetric case $Z_P \ll Z_T$ (or $Z_T \ll Z_P$).

The channel distortion applied in the CDW method is not significant enough to induce rearrangement on its own. It is accordingly not qualified as a substantial distortion, but it does lead to a series expansion with a connected kernel. While there are no obvious difficulties with the formal convergence properties of the CDW series, the question is to what extent the connectedness is set up by nonphysical forces which would have to be compensated for by higher-order terms. That this is a problem in the CDW method is documented by the pathological behavior of the first CDW approximation in the Thomas peak region.

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APPENDIX A

In this appendix we consider the distorted-wave formulation with the partitioning

$$V_i = V_P = U_i + W_i \ , \tag{A1}$$

where the distortion potential U_i and the residual potential W_i are given by

$$U_i = V_P - V_T G_0^{+} V_P \tag{A2}$$

and

$$W_i = V_T G_0^{+} V_P \ . \tag{A3}$$

Using a standard resolvent-operator identity it is seen that the corresponding distorted-wave Green's operator, defined in Eq. (13), satisfies the integral equation

$$g_i^{+} = G_P^{+} + g_i^{+} V_T G_0^{+} \ . \tag{A4}$$

Applying this identity in the distorted-wave Møller operator ω_i^{+} defined in Eq. (12) it is readily found that

$$\omega_i^{+} = 1 + G_P^{+} V_P = \omega_P^{+} \ . \tag{A5}$$

This expression is identical to the operator which generates the SPB scattering states in the strong projectile case [see Eq. (32)]. A similar relation is readily derived for the final channel.

APPENDIX B

It is shown that the CDW waves (61) are asymptotically orthogonal to the undistorted waves with respect to the rearranged channel, i.e., that overlap matrix elements such as $\langle \chi_f^{-(\mathrm{CDW})} \mid \Phi_i \rangle$ are bounded. This in turn implies that the distortion part of the distorted-wave T matrix [Eqs.

(14) and (15)] vanishes in the CDW case.

First we establish a simple relation between the overlap matrix element and the corresponding prior form of the T matrix in the PIA (Ref. 26) [equivalent to the continuum intermediate state (CIS) approximation[27]],

$$T_{if}^{\mathrm{PIA}} = \langle \chi_f^{-(\mathrm{CDW})} \mid V_P \mid \Phi_i \rangle \ . \tag{B1}$$

The relation is derived by performing a Fourier analysis of the electron coordinate dependence ($\mathbf{r}_P$) in $\chi_f^-(\mathbf{r}_P,\mathbf{R}_P)$. Upon switching to Jacobi coordinates ($\mathbf{r}_T,\mathbf{R}_T$) and performing the integrations over $\mathbf{R}_T$ we obtain the identity

$$\langle \chi_f^{-(\mathrm{CDW})} \mid \Phi_i \rangle = -\frac{2}{K^2+(Z_P/n_f)^2} T_{if}^{\mathrm{PIA}} \ , \tag{B2}$$

where $\mathbf{K}$ is the momentum transfer $\mathbf{K}\cong\mathbf{K}_f-\mathbf{K}_i$, and n_f is the principal quantum number of the hydrogenlike final state.

The overlap matrix element (B2) is certainly bounded since T^{PIA} is not known to possess singularities on the energy shell. This may be directly verified using explicit expressions[3] for T^{PIA}.

APPENDIX C

In this appendix we reduce the approximate second-order part of the CDW2 given in Eq. (65) to the six-dimensional integral in Eq. (67). Considering the matrix elements in the integrand on the rhs of Eq. (65) we may introduce Coulomb continuum functions in momentum space $\tilde{\phi}_{\mathbf{k}}^{\pm}(\mathbf{k})$ to obtain, with $\alpha=M_T(M_T+m_e)^{-1}$ and $\beta=M_p(M_p+m_e)^{-1}$,

$$\langle \Phi_{\mathbf{p},\mathbf{P}} \mid W_i \mid \chi_i^{+(\mathrm{CDW})} \rangle = (\mathbf{K}_i-\mathbf{P})\cdot[p-\alpha(\mathbf{K}_i-\mathbf{P})]\tilde{\phi}_i(\mathbf{p}-\alpha(\mathbf{K}_i-\mathbf{P}))\tilde{\phi}^{\,+}_{\mathbf{v}}(\mathbf{K}_i-\mathbf{P}-\mathbf{v}) \tag{C1}$$

and

$$\langle \chi_f^{-(\mathrm{CDW})} \mid W_f^{\dagger} \mid \Phi_{\mathbf{p},\mathbf{P}} \rangle = (\mathbf{p}+\alpha\mathbf{P}-\mathbf{K}_f)\cdot(\beta\mathbf{K}_f-\mathbf{P})\tilde{\phi}_f^{\,*}(\beta\mathbf{K}_f-\mathbf{P})\tilde{\phi}_{\mathbf{v}}^{\,-*}(\mathbf{p}+\alpha\mathbf{P}-\mathbf{K}_f+\mathbf{v}) \ . \tag{C2}$$

The momentum-space Coulomb wave functions have been evaluated by Guth and Mullin.[28] At high velocities it is sufficient to include the leading terms in powers of $\nu=Z/k$ as given by Bethe and Salpeter[29] [Eq. (9.13)], i.e.,

$$\tilde{\phi}_{\mathbf{k}}^{\pm}(\boldsymbol{\kappa}) = (2\pi)^{3/2}\{\delta^3(\boldsymbol{\kappa}-\mathbf{k}) + 2\tilde{V}_c(\boldsymbol{\kappa}-\mathbf{k})[(k-\kappa\pm i\eta)(k+\kappa)]^{-1}\} \ , \tag{C3}$$

where $\tilde{V}_c(\boldsymbol{\kappa})$ is the Fourier transform of the Coulomb potential. Since $x\delta(x)=0$, the first term on the rhs of (C3) does not contribute in Eqs. (C1) and (C2). Then we find, for $\nu_P=Z_P/v\ll 1$,

$$\langle \Phi_{\mathbf{p},\mathbf{P}} \mid W_i \mid \chi_i^{+(\mathrm{CDW})} \rangle = (2\pi)^{-3/2}\frac{(\mathbf{K}_i-\mathbf{P})\cdot[\mathbf{p}-\alpha(\mathbf{K}_i-\mathbf{P})]}{(v+\mid \mathbf{K}_i-\mathbf{P}-\mathbf{v}\mid)(v-\mid \mathbf{K}_i-\mathbf{P}-\mathbf{v}\mid +i\epsilon)}\tilde{V}_P(\mathbf{K}_i-\mathbf{P})\tilde{\phi}_i(\mathbf{p}-\alpha(\mathbf{K}_i-\mathbf{P})) \tag{C4}$$

and, correspondingly, for $\nu_T=Z_T/v\ll 1$,

$$\langle \chi_f^{-(\mathrm{CDW})} \mid W_f^{\dagger} \mid \Phi_{\mathbf{p},\mathbf{P}} \rangle \cong (2\pi)^{-3/2}\frac{(\beta\mathbf{K}_f-\mathbf{P})(\mathbf{p}+\alpha\mathbf{P}-\mathbf{K}_f)}{(v+\mid \mathbf{p}+\alpha\mathbf{P}-\mathbf{K}_f+\mathbf{v}\mid)(v-\mid \mathbf{p}+\alpha\mathbf{P}-\mathbf{K}_f+\mathbf{v}\mid -i\epsilon)}\tilde{V}_T(\mathbf{p}+\alpha\mathbf{P}-\mathbf{K}_f)\tilde{\phi}_f^{\,*}(\beta\mathbf{K}_f-\mathbf{P}) \ . \tag{C5}$$

Inserting (C4) and (C5) in Eq. (65) now leads, after a change of variables

$$\mathbf{q}=\mathbf{p}-\alpha(\mathbf{K}_i-\mathbf{P}), \quad \mathbf{k}=\beta\mathbf{K}_f-\mathbf{P} \ ,$$

and an expansion in (m_e/M), to Eq. (67).

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