Coupled equations for medium-energy scattering. I

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A simple set of coupled equations applicable for medium-energy scattering by composite systems is derived. The scattering function is expanded in the basis functions such that the average inelastic scattering channels simulate both adiabatic and impulse limits. Detailed discussions are given on the construction of the basis functions by the sum-rule technique. A procedure to solve the coupled set of equations by the Green's functions is presented, and the evaluation of the amplitude using the angle-averaging method is outlined.

I. INTRODUCTION

The coupled-channel method (CCM) has been used[1,2] widely in scattering problems of composite systems, often yielding reliable amplitudes whenever a small number of channels dominate the particular process. Sometimes, simple forms of effective distortion potentials are also introduced within the CCM scheme to simulate the effect of those channels which are neglected. In fact, some of the channels included in the CCM need not correspond to any specific physical states, and, among others, the pseudostate expansions[3-5] and effective-channel methods[6,7] have also been considered. The CCM automatically takes into account the nonlocal, energy-dependent, and absorptive characters of the process inherent in the effective potentials[8,9] for the composite-system scattering. Furthermore, iterative solutions of the coupled equations describe the rescattering effect in a very natural way.

Once a set of coupled equations is derived by reducing the original multichannel, many-particle scattering problem, the task of solving it is usually a well-defined and straightforward problem. However, such a reduction is by no means unique and depends very much upon the way basis functions are chosen. It is the purpose of this paper to describe an approach for the construction of a set of equations which is reasonably simple to solve and yet contains enough important features which are needed to treat *both* low- and high-energy collisions. The essential part of the physics is put in through careful choices of the basis functions, while the relative importance of the various terms will be decided optimally by the coupled equations themselves.

For a scattering of incoming distinguishable particles by a composite target, described by

$$H = T(\vec{R}) + H_T(\vec{r}) + V(\vec{r},\vec{R}) , \tag{1.1}$$

the scattering function is often expanded in terms of the undistorted target functions $\{\psi_n(\vec{r})\}$ and the resulting series truncated, as

$$\Psi(\vec{r},\vec{R}) = \sum_{n=0} \psi_n(\vec{r}) u_n(\vec{R}) \approx \sum_{n=0}^{N} \psi_n(\vec{r}) u_n(\vec{R}) , \tag{1.2}$$

where

$$H_T(\vec{r})\psi_n(\vec{r}) = E_{Tn}\psi_n(\vec{r}) . \tag{1.3}$$

When a large number of such states are involved collectively, the truncated form (1.2) is not very useful, and other approaches are needed. Thus, at low energies, for example, the polarized-orbital method[10] takes the form

$$\Psi \approx [\psi_0(\vec{r}) + \varphi_{\rm pol}(\vec{r},\vec{R})]\, u_0(\vec{R}) , \tag{1.4}$$

or its extensions

$$\Psi \approx [\psi_0(\vec{r}) + c\varphi_{\rm pol}(\vec{r},\vec{R})]\, u_0(\vec{R}) , \tag{1.5}$$

$$\Psi \approx \psi_0(\vec{r}) u_0(\vec{R}) + \varphi_{\rm pol}(\vec{r},\vec{R})\omega(\vec{R}) , \tag{1.6}$$

where $\varphi_{\rm pol}(\vec{r},\vec{R})$ is determined, e.g., from the equation

$$[H_T(\vec{r}) - E_{T0}]\,\varphi_{\rm pol} = -QV\psi_0(\vec{r}). \tag{1.7}$$

In (1.7), we have used the projections

$$Q = 1 - P, \quad P = |\psi_0(\vec{r})\rangle\langle\psi_0^*(\vec{r}')| . \tag{1.8}$$

Incidentally, (1.5) and (1.6) give bounds on the resulting amplitudes, while (1.4) does not, because both c and ω are to be varied *optimally* for a given $\varphi_{\rm pol}$. In general, (1.7), which is the sum-rule technique resulting from the second-order perturbation theory, is a difficult equation to solve, and various simpler versions are often used. In the form (1.6), the ω channel simulates all the Q-space effect through a single function $\varphi_{\rm pol}$. The pseudostate method[3-5] is a direct generalization of (1.6),

in which a set of basis functions $\{\varphi_{nt}\}$ are predetermined (although this is not necessary at low energies), from H_T or H_T+V, and the scattering function Ψ is then expanded in the form

$$\Psi \approx \psi_0 u_0 + \sum_{n=1}^{N} \varphi_{nt}\,\omega_n \ . \tag{1.9}$$

Note that φ_{nt} in (1.9) need not necessarily correspond to any physical channels. At low energies, (1.9) has proven to be an extremely powerful way of accurately solving many-particle scattering problems.[4,11]

As the scattering energy increases, other terms in H become as important as H_T, and the methods described above are not very effective, as they single out H_T or H_T+V as the dominant part of H at low energies. In fact, at extremely high energies, the operator T or $T+V$ plays a more prominent role. For example, the Glauber approximation[12] on the scattering function

$$\Psi \approx e^{i\vec{K}_0\cdot\vec{R}}\psi_0(\vec{r})\Phi_G \equiv \Psi_G, \tag{1.10}$$

where

$$\Phi_G = \exp\left(-\frac{i}{K_0}\int_{-\infty}^{Z} V(\vec{r},\vec{R}')\,dZ'\right),\quad R' = (b^2+Z'^2)^{1/2}\ , \tag{1.11}$$

has proven to be very effective in atomic[13] and nuclear[14] problems. However, (1.10) has its drawbacks; its validity breaks down either (a) at large angles[15] (or momentum transfer), or (b) when the effect of the target bindings becomes important. As the scattering energy decreases, these difficulties become serious.

For medium-energy scatterings of interest here, neither the forms such as (1.6) nor (1.10) is satisfactory. Thus, for example, a slightly different approach was discussed by Mittleman[16] recently, in which Ψ is written as

$$\Psi \approx \psi_0(\vec{r})u_0(\vec{R}) + \varphi(\vec{r})\omega(\vec{R})\ , \tag{1.12}$$

where u_0, φ, and ω are all unknown functions to be determined by a set of three coupled equations. However, the resulting equations satisfied by these functions are extremely complicated and nonlinear, so that it is probably a hopeless job to solve them with any reasonable accuracy. In view of the discussions given above, we propose here an alternate expansion of Ψ, which incorporates *both* features of (1.6) and (1.10) but avoids the complication of (1.12).

II. COUPLED EQUATIONS

For the medium-energy scattering of interest here, the forms (1.6), (1.10), and (1.12) are not suitable by themselves, but we can certainly combine them with proper coefficient functions and optimize them by solving the resulting coupled equations. Thus, we write

$$\Psi(\vec{r},\vec{R}) \approx \psi_0(\vec{r})u_0(\vec{R}) + \varphi_t(\vec{r},\vec{R})\omega(\vec{R}) + \chi(\vec{r})y_t(\vec{R},\vec{r})\ , \tag{2.1}$$

where the basis functions $\psi_0(\vec{r}), \varphi_t$, and y_t are assumed known, while u_0, ω, and χ are to be obtained from a set of three coupled equations. As in (1.6) and (1.10), φ_t will describe the adiabatic component of Ψ and y_t is for the impulse part. Presumably, at low energies, the ω "channel" will dominate while at high energies the y_t "channel" will be more important. In fact, the form (2.1) with $\varphi_t = 0$ would be a significant improvement over (1.10), especially at large angles, and deserves further study.

The basis functions may be obtained in a variety of ways. Here, as with (1.7), we apply the perturbative sum-rule technique and write, for example,

$$(H_T - E_{T0})\varphi_t(\vec{r},\vec{R}) = -QV\psi_0(\vec{r}) \tag{2.2}$$

for the low-energy part of the contribution in Ψ, and[15]

$$(T - E_y')y_t(\vec{R},\vec{r}) = -(V - \langle V\rangle_{\vec{R}})e^{i\vec{K}_0\cdot\vec{R}} \tag{2.3}$$

for the high-energy part of Ψ. In (2.3), we have introduced

$$\langle V\rangle_{\vec{R}} \equiv \int d\vec{R}\, V(\vec{r},\vec{R})e^{i\vec{q}\cdot\vec{R}},\quad \vec{q} = \vec{K}_0 - \vec{K}_f \tag{2.4}$$

where $\vec{K}_0$ is the initial particle momentum and $\vec{K}_f$ the final state momentum. [See Appendix A for an alternative to (2.3).] In the extreme-high-energy limit, (2.3) is what one would obtain in the impulse approximation of the Glauber type.[12] The additional term in (2.3), which is proportional to $\langle V\rangle_{\vec{R}}$, is included to minimize the double counting of the effect of V in the u_0 term. The property of (2.2) and (2.3) will be discussed in more detail in Sec. III, but we should stress the fact that they are very convenient but not a unique choice. Obviously, by construction, (2.1) will go over to the forms appropriate at low- and at high-energy limits, and thus it is reasonable to expect that the medium-energy scattering may also be treated effectively by (2.1), if and only if the coupled equations are solved to determine the coefficient functions.

Substitution of (2.1) into the scattering equations and operating with

$$\int d\vec{r}\,\psi_0^*(\vec{r}),\ \int d\vec{r}\,\varphi_t^*(\vec{r},\vec{R}),\ \text{and}\ \int d\vec{R}\, y_t^*(\vec{R},\vec{r}) \tag{2.5}$$

in the usual way, we obtain the following set of

coupled equations for u_0, ω, and χ; noting the unusual variable change in the last integration, we have firstly for u_0,

$$(T+V_{00}-E_0')u_0(\vec{R}) = -V_{0\varphi}\omega - V_{0y}\chi, \tag{2.6}$$

where

$$V_{00} = \int d\vec{r}\,|\psi_0|^2 V(\vec{r},\vec{R}) \equiv \langle V\rangle_r^{\rightarrow}, \tag{2.7a}$$

$$E_0' = E - E_{T0},$$

and, in the symbolic notation,

$$V_{0\varphi} = \int d\vec{r}\,\psi_0^*(\vec{r})(H-E)\varphi_t(\vec{r},\vec{R}) = \int d\vec{r}\,\psi_0^*(\vec{r})V\varphi_t(\vec{r},\vec{R}), \tag{2.7b}$$

$$V_{0y}\chi \equiv \int d\vec{r}\,\psi_0^*(\vec{r})(H-E)\chi(\vec{r})y_t(\vec{R},\vec{r}). \tag{2.7c}$$

In (2.7b), we used the fact that φ_t is in the Q space orthogonal to ψ_0, and V_{0y} in (2.7c) is essentially an integral operator on the unknown function χ. (The function χ could be obtained under the constraint that it is also in the Q space, orthogonal to ψ_0, in a simpler case when y_t is taken to be independent of the $\vec{r}$ variable. But, we do not consider this possibility here.)

The equation satisfied by ω is similar to (2.6) but more involved because of the $\vec{R}$ dependence of $\varphi_t(\vec{r},\vec{R})$. Although φ_t is uniquely given, e.g., by (2.2) so that its normalization is not arbitrary, the fact that φ_t is multiplied by an unknown coefficient function ω in (2.1) allows one to have

$$\int |\varphi_t|^2 d\vec{r} = 1,$$

for all values of $\vec{R}$. That is, the normalized φ_t is the same as the earlier one, with a function of the $\vec{R}$ variable multiplied. Then, we have

$$(T+V_{\varphi\varphi}+J_{\varphi\varphi}-E_\varphi')\omega(\vec{R}) = -V_{\varphi 0}u_0 - V_{\varphi y}\chi, \tag{2.8}$$

where

$$V_{\varphi\varphi} = \int d\vec{r}\,|\varphi_t|^2 V(\vec{r},\vec{R}), \tag{2.9a}$$

$$J_{\varphi\varphi} = \int d\vec{r}\,\varphi_t^* T(\vec{R})\varphi_t, \tag{2.9b}$$

$$E_\varphi'(\vec{R}) = E - \int d\vec{r}\,\varphi_t^* H_T \varphi_t \equiv E - \bar{E}_\varphi(\vec{R}), \tag{2.9c}$$

and

$$V_{\varphi 0} = \int d\vec{r}\varphi_t^* V\psi_0 = V_{0\varphi}^*, \tag{2.9d}$$

$$V_{\varphi y}\chi \equiv \int d\vec{r}\varphi_t^*(H-E)\chi y_t. \tag{2.9e}$$

First of all, in $V_{\varphi\varphi}$, the $\vec{R}$ dependence comes both from φ_t and V, just as in the adiabatic formulation of slow-collision processes. The $J_{\varphi\varphi}$ term also arises from the R dependence of φ_t and may not be negligible in the medium- and high-energy scattering, although it is generally negligible at low energies. E_φ' depends on the R variable, and, in the limit $R\to\infty$, $\bar{E}_\varphi$ will approach a constant *average excitation energy* of the target. It is real for all R and approaches a value higher than E_{T0}, since φ_t is in the Q space. The $V_{\varphi y}$ is an integral operator acting on χ while y_t is a known function of both $\vec{r}$ and $\vec{R}$ variables.

Finally, we consider the equation satisfied by χ. It is in the $\vec{r}$ variable, where $\vec{r} = (\vec{r}_1 \cdots \vec{r}_A)$ is the internal-target variable for A particles. Since y_t is not normalizable in the usual sense, we could introduce a convergent factor $e^{-\gamma R}$ in (2.5) for the $d\vec{R}$ integration and may let $\gamma \to 0$ at the end. Thus,

$$[H_T(\vec{r}) + U_{yy}(\vec{r}) + J_{yy} - E_y]\chi(\vec{r}) = -U_{y0}u_0 - U_{y\varphi}\omega, \tag{2.10}$$

where

$$U_{yy} = \int d\vec{R}\,|y_t|^2 e^{-\gamma R} V(\vec{r},\vec{R})/D_y, \tag{2.11a}$$

$$J_{yy}\chi \equiv \left(\chi(\vec{r})\int d\vec{R}\,e^{-\gamma R} y_t^* H_T y_t - \frac{\hbar^2}{m}\sum_{i=1}^{A}(\vec{\nabla}_{\vec{r}_i}\chi)\cdot\int d\vec{R}\,y_t^*\vec{\nabla}_{\vec{r}_i} y_t\, e^{-\gamma R}\right)\Big/ D_y, \tag{2.11b}$$

$$E_y = E - \int d\vec{R}\,e^{-\gamma R}(y_t^* T y_t)/D_y \equiv E - \bar{E}_y(\vec{r}), \tag{2.11c}$$

and

$$U_{y0}u_0 \equiv \psi_0(\vec{r})\int d\vec{R}\,y_t^*(\vec{R},\vec{r})e^{-\gamma R} \times (T+V-E_0')u_0(\vec{R})/D_y^{1/2}, \tag{2.11d}$$

$$U_{y\varphi}\omega \equiv \int d\vec{R}\,y_t^*(\vec{R},\vec{r})e^{-\gamma R}(H-E)\varphi_t(\vec{r},\vec{R})\omega/D_y^{1/2}, \tag{2.11e}$$

with

$$D_y(\vec{r}) = \int d\vec{R}\,e^{-\gamma R}|y_t|^2. \tag{2.11f}$$

Again U_{y0} and $U_{y\varphi}$ are integral operators acting on u_0 and ω, respectively. This came about, as with V_{0y} and $V_{\varphi y}$, because of the variable switch between $\vec{r}$ and $\vec{R}$ in the last term of (2.1). The J_{yy} term is expected to be small at high energies, as $J_{\varphi\varphi}$ in the low-energy limit, but may not be

negligible as the scattering energy decreases.

The equations (2.6), (2.8), and (2.10) are the desired set of coupled equations. The analogy between the low- and high-energy parts is obvious. The equations are *linear* in the three unknown functions u_0, ω, and χ, so that their solution can be obtained without the complexity and instability arising from the nonlinearity. Instead of formally solving this set of equations and uncoupling them to obtain an effective interaction in the elastic channel, for example, we briefly consider several simpler cases of the present formalism.

(i) The expansion (2.1) is the most general form involving three-term expansion. To simplify the calculation, φ_t and y_t may be replaced by $\varphi_t(\vec{r})$ and $y_t(\vec{R})$, respectively, so that the dependence on the parametric variables is absent. This reduces (2.2) and (2.3) such that the inhomogeneous terms have to be zero. The resulting expansion of Ψ is

$$\Psi \approx \psi_0(\vec{r})u_0(\vec{R}) + \sum_{\alpha=1}^{N_\alpha} \varphi_{t\alpha}(\vec{r})\omega_\alpha(\vec{R}) + \sum_{\beta=1}^{N_\beta} \chi_\beta(\vec{r})y_{t\beta}(\vec{R}), \tag{2.12}$$

where we have added more than one term of each kind, resulting in $N_\alpha + N_\beta + 1$ coupled equations, and where $\varphi_{t\alpha}$ may be determined from $H_T + \overline{U}(r)$, e.g., and $y_{t\beta}$ by $T + \overline{V}(R)$. $\overline{U}$ and $\overline{V}$ are some reasonably chosen distortion potentials. The form (2.12) is a direct generalization of the pseudostate expansion, in which the last sum is added.

(ii) We can mix in the features of (2.12) with (2.1) and write, e.g.,

$$\Psi \approx \psi_0 u_0 + \varphi_t(\vec{r}, \vec{R})\omega(\vec{R}) + \sum_{\beta=1}^{N_\beta} \chi_\beta(\vec{r})y_{t\beta}(\vec{R}), \tag{2.13a}$$

or

$$\Psi \approx \psi_0 u_0 + \sum_{\alpha=1}^{N_\alpha} \varphi_{t\alpha}(\vec{r})\omega_\alpha(\vec{R}) + \chi(\vec{r})y_t(\vec{R}, \vec{r}). \tag{2.13b}$$

(iii) Even simpler approaches are to directly extend the low- or high-energy techniques toward the medium-energy region using

$$\Psi \approx \psi_0 u_0 + \varphi_t(\vec{r}, \vec{R})\omega(\vec{R}) \tag{2.14a}$$

or

$$\Psi \approx \psi_0 u_0 + \chi(\vec{r})y_t(\vec{R}, \vec{r}). \tag{2.14b}$$

For medium energy, slow collisions, as in the ion-atom scattering, (2.14a) should still be a reasonable form, while (2.14b) should be better for lighter-particle scattering such as in the electron-atom collision.

We add two remarks concerning the coupled equations formulated above. Firstly, we note that the χ equation is still an A-body problem of the target system, so that it is not reasonable to ask for its exact solution. For $A \geq 2$, we are forced again to introduce approximations. We simply mention the possibility of solving the χ equation by a *variational* procedure. In that case, we have a variational iteration procedure, in which u_0 and ω are treated as they are in (2.6) and (2.8), but χ is solved variationally in an iterative way.

Secondly, we should also consider the case of inelastic, exchange and rearrangement collisions. Unlike a formulation of the theory in which H is modified in some approximate ways, we have formulated the problem in terms of the wave-function construction. Therefore, it is almost trivial to modify (2.1) such that the above complications can be taken into account; i.e., we simply include the proper symmetrization and additional terms in Ψ, without changing the basic structure of (2.1). The problems of overcompleteness and nonorthogonality present no difficulties,[17] as they have been fully discussed earlier.

III. BASIS FUNCTIONS

We return to (2.2) and (2.3), and consider in more detail various approximations which may be introduced to evaluate the basis functions φ_t and y_t which appear in (2.1). As stressed earlier, the forms (2.2) and (2.3) are not necessarily the optimum choice, but are simple because the right-hand sides are taken to be the known functions obtained from the lowest-order perturbation theory. We can illustrate the approximations involved by studying the original effective potential in the elastic channel. Following Feshbach,[8] we have the effective potential for the elastic scattering given by

$$U_{el} = (\psi_0, V\psi_0)_{\vec{r}} + (\psi_0, VG^Q V\psi_0)_{\vec{r}}, \tag{3.1}$$

where

$$G^Q = [Q(E + i\epsilon - H)Q]^{-1}. \tag{3.2}$$

Obviously, for a simple form of G^Q, the elastic amplitude can be calculated rather trivially. Thus, the problem is to evaluate G^Q. We will show that (2.2) and (2.3) are in fact simple approximations to G^Q in the respective limits.

A. Adiabatic function $\varphi_t(\vec{r};\vec{R})$

Explicitly, (2.2) is

$$(H_T - E_{T0})\varphi_t(\vec{r}, \vec{R}) = -(V - \langle V \rangle_{\vec{r}})\psi_0(\vec{r}), \tag{3.3}$$

where

$$\langle V \rangle_{\vec{r}} = \int d\vec{r}\, |\psi_0|^2 V(\vec{r}, \vec{R}) \equiv V_{00}.$$

Equation (3.3) may be formally solved as

$$\varphi_t(\vec{r},\vec{R}) = \int d\vec{r}\,' G_T^Q(\vec{r},\vec{r}\,')V(\vec{r}\,',\vec{R})\psi_0(\vec{r}\,') , \quad (3.4)$$

with

$$G_T^Q = [Q(E_{T0} - H_T)Q]^{-1}.$$

On the other hand, from (3.1), we see that the adiabatic expansion[18]

$$G^Q = G_T^Q + G_T^Q(T + V - E_0')G_T^Q + \cdots \quad (3.5)$$

provides (3.4) as the lowest-order term in which the motion of the projectile is neglected. The sum-rule technique then asserts that, to evaluate φ_t, we do not use G_T^Q in (3.4) but simply solve (3.3) directly for φ_t.

Equation (3.3) is still an A-body problem in the external field provided by the stationary particle at $\vec{R}$, and is a difficult equation to solve. In low-energy applications, the partial-wave expansion of φ_t is usually made, owing to the importance of the long-range forces coming from the few low partial waves, and then a few low-angular-momentum states are evaluated.[10] Such a procedure may not be effective at higher energies, and we consider here two simple alternatives. The first possibility is to use the *closure* approximation and set

$$G_T^Q \approx \frac{Q}{E_{T0} - \bar{E}_T} \quad (3.6)$$

and thus

$$\varphi_t \approx \frac{1}{E_{T0} - \bar{E}_T} QV\psi_0 = \frac{(V - \langle V\rangle_{\vec{r}})\psi_0}{E_{T0} - \bar{E}_T} , \quad (3.7)$$

where the average energy $\bar{E}_T$ may be calculable by studying the target system alone. Equation (3.7) may be a reasonable approximation if many Q states contribute collectively.

Note that in the approximation (3.7), the factor $(E_{T0} - \bar{E}_T)^{-1}$ may be dropped since such a factor, and the normalization of φ_t at each fixed R, can always be absorbed into an unknown function ω. Therefore, the form (3.7) has the additional feature that φ_t is obtained very trivially without unknown parameters such as $\bar{E}_T$. In fact, the form[7]

$$\varphi_t\,\omega \sim QVP\Psi^P ,$$

where $P\Psi^P$ satisfes $P(H - E)P\Psi^P = 0$, was used earlier in the estimate of $\bar{E}_T$ itself.

The second and more ambitious approach on φ_t is to set up a variational calculation using a functional

$$[J] \equiv 2(Q\varphi_t, V\psi_0) + (Q\varphi_t(H_T - E_{T0})Q\varphi_t), \quad (3.8)$$

where $[J]$ is negative definite. Note that (3.8) is slightly different from a variational estimate on G_T^Q, as

$$G_T^Q \leqslant G_{Tt}^Q \leqslant 0,$$

where

$$G_{Tt}^Q = \sum_{\alpha,\beta=1}^{N} |Q\psi_{t\alpha}\rangle[(Q\psi_{t\alpha'}, \times(E_{T0} - H_T)Q\psi_{t\beta'})^{-1}]_{\alpha\beta}\langle Q\psi_{t\beta}| .$$

Incidentally, it is also of interest to point out that one can obtain a finite set of $\varphi_{\alpha t}(\vec{r},\vec{R})$ by diagonalizing the matrix formed with $H_T + V$ and trial functions, which generates a set of molecular pseudostates.[19]

B. Impulse function y_t

While the φ_t term takes care of the adiabatic part of the collision, y_t is specifically designed to represent the high-energy component in Ψ. Thus, it is reasonable to solve (2.3) in the high-energy impact-parameter representation. As in (2.2), the term $\langle V\rangle_{\vec{R}}$ in the right-hand side of (2.3) is included to minimize the double counting of the effect of V in u_0, although this problem will be eliminated automatically when the coupled equations for u_0, ω, and χ are solved. In the high-energy limit, the projectile assumes nearly straight-line trajectory and we may rewrite (2.3) in the cylindrical coordinates, with $\vec{K}_0$ along the $\hat{z}$ direction. Then, with $E_y' \approx E_0' = \hbar^2K_0^2/2M$, we have

$$y_t(\vec{R},\vec{r}) = \int d\vec{R}\,' g_0(\vec{R},\vec{R}')[V - \langle V\rangle_{\vec{R}}]e^{i\vec{K}_0\cdot\vec{R} - \gamma R'} , \quad (3.9)$$

where

$$g_0(\vec{R},\vec{R}') = (E_0' + i\epsilon - T)^{-1} = -\frac{2M}{4\pi|\vec{R} - \vec{R}'|}e^{iK_0|\vec{R} - \vec{R}'|}$$

or

$$g_0 \approx -\frac{2M\delta(\vec{b} - \vec{b}')}{4\pi|z - z'|}e^{iK_0|z - z'|} \approx g_0^{\text{eik}} , \quad (3.10)$$

where

$$g_0^{eik} = -(i/K_0)e^{i\vec{K}_0\cdot(\vec{R} - \vec{R}')}\delta(\vec{B} - \vec{B}')\theta(z - z') .$$

The convergence factor $e^{-\gamma R}$ is included in (3.9) (with $\gamma \to 0$ at the end of the integrations). As expected, the $\langle V\rangle_{\vec{R}}$ term in (3.9) subtracts out from g_0 that part of the state which is proportional to $e^{i\vec{K}_f\cdot\vec{R}}$, as (2.4) shows that $\langle V\rangle_{\vec{R}}$ is in general momentum-transfer dependent. With the eikonal approximation (3.10), however, we may set $\vec{q} = 0$ in $\langle V\rangle_{\vec{R}}$. (For scatterings at large angles, with $\vec{q} \neq 0$, the original exact g_0 may be kept without the straight-line approximation.)

The connection between g_0 and G^Q in (3.1) can be seen from the series

$$G^Q = Qg_0Q + g_0Q(H_T + V - E_{T0})Qg_0 + \cdots . \quad (3.11)$$

Thus, y_t of (2.3) completely neglects the target structure, but includes the interaction V to first order, with the target particles fixed at $\vec{r} = (\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A)$. This is precisely the scattering picture represented by the Glauber approximation,[12] especially when g_0^{eik} is inserted in y_t for g_0. Presumably, (3.9) should give an improved amplitude at large angles as g_0 contains the outgoing waves in all directions. On the other hand, the role of $\langle V\rangle_{\vec{R}}$ in (3.9) is yet to be clarified by more detailed analyses. Somewhat different forms for the basis function y_t are studied in Appendix A. The prevailing theme in the construction of the basis functions is that, although they essentially determine the goodness of the resulting amplitudes, their form should be simple and compact. The form (3.7) for φ_t is preferable in this respect and we have for y_t

$$y_t \approx (V - \langle V\rangle_{\vec{r}}) e^{i\vec{K}_0\cdot\vec{R}} \equiv \hat{y}_t , \tag{3.12}$$

as given in (A6), where the unknown parameter which results from the closure approximation is absorbed in the function χ.

We have seen above that the basis functions φ_t and y_t are designed to represent the two extreme physical pictures of the composite-system scattering, and they assume the complementary role in the wave function (2.1); the relative importance of the two terms is determined automatically through their coefficient functions ω and χ, when the coupled equations are solved. In this way, the main difficulty of formulating the medium-energy scattering problem can be treated without the prior knowledge of the effectiveness of either term.

The above discussion does not preclude the possibility of employing the less ambitious forms (2.14), which are simpler, but naturally less effective, than (2.1). Nevertheless, the resulting amplitudes may be a significant improvement over the form such as that given by (1.10). The form (2.14a), for example, gives rise to a formulation which is very closely related to the effective-channel theory of Refs. 6 and 7 for the high-energy nuclear reactions. As mentioned earlier, the approach with (2.14a) has the advantage that the theory is well-defined once the function φ_t is chosen. The exchange effect, which is known to be negligible at high energies,[9] may become important at lower energies, and a simple symmetrization of (2.14a) as

$$\Psi = [\psi_0(\vec{r})\, u_0(\vec{r}_0) + \varphi_t(\vec{r}, \vec{r}_0)\, \omega(\vec{r}_0)] + \sum_{i=1}^{A} \epsilon_{\pm}(\vec{r}_0 - \vec{r}_i)[\cdots] \tag{3.13}$$

will be sufficient.

The effectiveness of (2.14b) has not yet been tested explicitly, but we give in Appendix B the leading correction to the Glauber amplitude coming from the target-structure contribution.

IV. ELASTIC SCATTERING AMPLITUDE

The elastic scattering amplitude is constructed using the solution of the coupled equations derived in Sec. II. We consider here several ways of treating this problem, and, for definiteness, choose the set generated by (2.14a), i.e.,

$$(T + V_{00} - E_0')\, u_0(\vec{R}) = -\, V_{0\varphi}(\vec{R})\, \omega(\vec{R}) , \tag{4.1a}$$

$$(T + V_{\varphi\varphi} + J_{\varphi\varphi} - E_\varphi')\, \omega(\vec{R}) = -\, V_{\varphi 0}(\vec{R})\, u_0(\vec{R}) . \tag{4.1b}$$

The formal solution is obtained in terms of the Green's functions defined by

$$g_0^P(\vec{R}, \vec{R}') = (E_0' + i\epsilon - T - V_{00})^{-1} , \tag{4.2}$$

$$g_\varphi(\vec{R}, \vec{R}') = (E_\varphi' + i\epsilon - T - \overline{V})^{-1} , \tag{4.3}$$

where

$$\overline{V} \equiv V_{\varphi\varphi} + J_{\varphi\varphi} + \overline{E}_\varphi - E_\varphi' ,$$

$$E_\varphi' \equiv \lim_{R\to\infty} (E - \overline{E}_\varphi) ,$$

and the homogeneous solution

$$(T + V_{00} - E_0')\, u_0^P(\vec{R}) = 0 . \tag{4.4}$$

We then have

$$u_0 = u_0^P + g_0^P V_{0\varphi}\omega , \tag{4.5}$$

$$\omega = g_\varphi V_{\varphi 0} u_0 , \tag{4.6}$$

with the total wave function given by

$$\Psi_i \simeq \psi_0(\vec{r})\, u_0(\vec{R}) + \varphi_t(\vec{r}; \vec{R})\, \omega(\vec{R}) , \tag{4.7}$$

where

$$\varphi_t = (V - V_{00})\psi_0(\vec{r})/D_\varphi^{1/2} , \tag{4.8}$$

$$D_\varphi = \langle V^2\rangle_{\vec{r}} - \langle V\rangle_{\vec{r}}^2 .$$

The exact elastic amplitude is

$$\mathcal{T}_{el} = (\Phi_f,\, V\Psi_i)$$

$$= (\Phi_f,\, V\Phi_i) + (\Phi_f,\, VG\,V\Phi_i) , \tag{4.9}$$

where

$$\Phi_i \equiv \psi_0(\vec{r})\, e^{+i\vec{K}_i\cdot\vec{R}} \equiv \psi_0 u_i^{(0)} , \quad \vec{K}_i \equiv \vec{K}_0$$

$$\Phi_f \equiv \psi_0(\vec{r})\, e^{+i\vec{K}_f\cdot\vec{R}} \equiv \psi_0 u_f^{(0)} , \quad |\vec{K}_i| = |\vec{K}_f| \tag{4.10}$$

and

$$\Psi_i = \Phi_i + G\,V\Phi_i . \tag{4.11}$$

Note that the full Green's function G can be written[15] as

$$G \equiv (E + i\epsilon - H)^{-1} = G_{PP} + G_{PQ} + G_{QP} + G_{QQ} , \tag{4.12}$$

with

$$G_{PP}=[P(E+i\epsilon-H-VG^{Q}V)P]^{-1},$$
$$G_{PQ}=G^{P}PVQG_{QQ}, \tag{4.13}$$
$$G_{QP}=G^{Q}QVPG_{PP},$$
$$G_{QQ}=[Q(E+i\epsilon-H-VG^{P}V)Q]^{-1},$$

where

$$G^{P}=[P(E+i\epsilon-H)P]^{-1}.$$

For the total wave function of the form (4.7), we have

$$\begin{aligned}\mathcal{T}_{el}&\approx(\Phi_f,\ V(\psi_0 u_0+\varphi_t\omega))\\&=(u_f^{(0)},\ V_{00}u_0^{P})+(u_f^{(0)},\ V_{00}g_0^{P}V_{0\varphi}\omega)+(u_f^{(0)},\ V_{0\varphi}\omega)\\&\approx(u_f^{(0)},\ V_{00}u_0^{P})+(u_f^{(0)},\ V_{0\varphi}g_{\varphi}V_{\varphi 0}u_i^{(0)})\\&\equiv\mathcal{T}_{el}^{P}+\overline{\mathcal{T}}_{el}^{Q}.\end{aligned} \tag{4.14}$$

In (4.14), we have dropped all terms which involve more than one g_0^P or g_φ. This may be viewed as an approximation in (4.9) for G of the type

$$G_{PP}\approx Pg_0^{P}P,\quad G_{QQ}\approx Qg_{\varphi}Q,\quad G_{PQ}\approx G_{QP}\approx 0. \tag{4.15}$$

It is clear how the amplitude (4.14) could be improved further if necessary.

We evaluate u_0^P in $\mathcal{T}_{el}^P$ by two different ways. Firstly, the usual eikonal approximation with the straight-line trajectory gives[12]

$$u_0^{P}\approx e^{i\vec{K}_i\cdot\vec{R}}\exp\left(-\frac{i}{K_i}\int_{-\infty}^{z}V_{00}(R')dz'\right), \tag{4.16}$$

and thus

$$\mathcal{T}_{el}^{P}\approx 2\pi iK_i\int_0^{\infty}b\,db\,J_0(qb)(e^{i\chi^{P}(b)}-1), \tag{4.17}$$

where

$$\chi^{P}(b)=-K_i^{-1}\int_{-\infty}^{\infty}V_{00}(R')dz',$$
$$\vec{q}=\vec{K}_i-\vec{K}_f. \tag{4.18}$$

The amplitude $\mathcal{T}_{el}^P$ may also be evaluated using the Green's function g_0^P by first writing it in the form

$$\mathcal{T}_{el}^{P}=(u_f^{(0)},\ V_{00}u_i^{(0)})+(u_f^{(0)},\ V_{00}g_0^{P}V_{00}u_i^{(0)}). \tag{4.19}$$

The simplest form for g_0^P is given in the semiclassical approximation[20]

$$g_0^{P}(\vec{R},\vec{R})\approx-(2\pi)^{-1}e^{i\kappa^{P}(t)s}/s, \tag{4.20}$$

where

$$\vec{S}=\vec{R}-\vec{R}',\quad \vec{t}=\tfrac{1}{2}(\vec{R}+\vec{R}') \tag{4.21}$$

and

$$\kappa^{P}(t)=[2E_0'-2V_{00}(t)]^{1/2}=\text{real}. \tag{4.22}$$

The form (4.20) is simpler than the corresponding eikonal (WKB-type) form and was shown to be quite reliable.[20] Further simplification may be made by defining the new variables

$$s_z=|z-z'|,\quad t_z=\left[b^2+\left(\frac{z+z'}{2}\right)^2\right]^{1/2} \tag{4.23}$$

and set

$$g_0^{P}\approx-(2\pi)^{-1}\delta(\vec{b}-\vec{b}')e^{i\kappa^{P}(t_z)s_z}/s_z, \tag{4.24}$$

where the $\hat{z}$ axis is yet to be chosen. (Perhaps, $\hat{z}=\hat{K}_a$ below.)

The amplitude $\overline{\mathcal{T}}_{el}^{Q}$ is the leading correction to $\mathcal{T}_{el}^{P}$ and may be evaluated using g_φ of the form

$$g_{\varphi}\approx-(2\pi)^{-1}e^{i\kappa^{Q}(t)s}/s\equiv g_{\varphi}^{sc}, \tag{4.25}$$

where

$$\kappa^{Q}=[2E'_{\varphi}-2\overline{V}(t)]^{1/2}=\text{real} \tag{4.26}$$

or

$$g_{\varphi}\approx-(2\pi)^{-1}\delta(\vec{b}-\vec{b}')e^{i\kappa^{Q}(t_z)s_z}/s_z. \tag{4.27}$$

Thus, $\overline{\mathcal{T}}_{el}^{Q}$ becomes

$$\begin{aligned}\overline{\mathcal{T}}_{el}^{Q}\approx\int\int d\vec{t}\,d\vec{s}\,e^{i\vec{q}\cdot\vec{t}-i\vec{K}_a\cdot\vec{s}}g_{\varphi}^{sc}(s,t)\\\times V_{0\varphi}(\vec{t}-\tfrac{1}{2}\vec{s})V_{\varphi 0}(\vec{t}+\tfrac{1}{2}\vec{s}),\end{aligned} \tag{4.28}$$

with

$$\vec{K}_a=\tfrac{1}{2}(\vec{K}_i+\vec{K}_f). \tag{4.29}$$

A slightly simpler procedure than that involved in (4.28) is to go back to (4.1b) and consider a modified form of the equation

$$(T+\overline{V}-E'_{\varphi})\omega\approx-V_{\varphi 0}u_i^{(0)}. \tag{4.30}$$

If we set

$$\omega(\vec{R})\equiv e^{i\vec{K}'\cdot\vec{R}}e^{-i\overline{\chi}/\overline{K}}\vartheta(\vec{R}),$$

with $\vec{K}'=(2E'_{\varphi})^{1/2}$ and

$$\overline{\chi}=\int_{-\infty}^{z}\overline{V}(R')\,dz', \tag{4.32}$$

then $\vartheta(\vec{R})$ satisfies

$$\begin{aligned}[T-i\vec{K}\cdot\vec{\nabla}_{\vec{R}}+i(\overline{V}/\overline{K}^2)\vec{K}\cdot\vec{\nabla}_{\vec{R}}+\tilde{T}]\vartheta(\vec{R})\\=-V_{\gamma 0}e^{i(\vec{K}_i-\vec{K})\cdot\vec{R}}e^{+(i/\overline{K})\overline{\chi}},\end{aligned} \tag{4.33}$$

where

$$\tilde{T}\equiv e^{+i\overline{\chi}/\overline{K}'}Te^{-i\overline{\chi}/\overline{K}}. \tag{4.34}$$

Neglecting the terms T, $\tilde{T}$, and $\overline{V}/\overline{K}^2$, we obtain

$$\vartheta(\vec{R})\approx-\frac{i}{\overline{K}'}\int_{-\infty}^{z}dz'\,V_{\varphi 0}e^{i(\vec{K}_i-\vec{K})\cdot\vec{R}'}e^{i\overline{\chi}(R')/\overline{K}}, \tag{4.35}$$

and thus

$$\overline{\mathcal{T}}_{el}^{Q}\approx-\frac{i}{\overline{K}'}\int d\vec{b}\int_{-\infty}^{\infty}dz\,U_f^{*}(\vec{R})\int_{-\infty}^{z}U_i(\vec{R}')dz', \tag{4.36}$$

where

$$U_i(\vec{R}') = e^{i\vec{q}_i\cdot\vec{R}'} V_{0\varphi} e^{i\bar{X}'/\bar{K}}, \qquad U_f(\vec{R}) = e^{i\vec{q}_f\cdot\vec{R}} V_{0\varphi} e^{i\bar{X}/\bar{K}}, \tag{4.37}$$

and

$$\vec{q}_i \equiv \vec{K}_i - \vec{K}, \quad \vec{q}_f \equiv \vec{K}_f - \vec{K} \quad (\vec{q}_i - \vec{q}_f = \vec{q}). \tag{4.38}$$

The differential elastic scattering cross section is

$$\sigma_{el}(\theta) = \frac{1}{4\pi^2} |\mathcal{T}_{el}|^2, \tag{4.39}$$

where $\mathcal{T}_{el}$ is given, for example, by the sum of (4.17) and (4.36). A partial justification for (4.17), rather than (4.20), may be that many soft collisions do not require the transitions to the Q space, while the Q-space effect requires double hard collisions through $V_{0\varphi}$ and $V_{\varphi 0}$.

Obviously, both (4.19), with (4.20), for $\mathcal{T}^P_{el}$ and (4.28) for $\overline{\mathcal{T}}^Q_{el}$ each involve six-dimensional integrations corresponding to $d\vec{s}$ and $d\vec{t}$. However, the integrations will also be greatly simplified if we adopt the angle-averaging procedure developed recently.[15] It involves essentially a replacement of the angle-dependent term $\vec{t}\cdot\vec{s}$ in $V_{00}(\vec{R})V_{00}(\vec{R}')$ and in $V_{0\varphi}(\vec{R})V_{\varphi 0}(\vec{R}')$ by

$$\vec{t}\cdot\vec{s} \to \alpha_q ts, \tag{4.40}$$

where

$$\alpha_q = 1/\sqrt{3} \quad \text{or} \quad \alpha_q = (1/\sqrt{3})(1 - q/2K).$$

This procedure works for all forms of the potentials and has been shown recently[15] to work quite well for the range of q values much larger than that for the Glauber approximation. Except for a Gaussian form of the potential, an approximation such as (4.40) is unavoidable for the evaluation of the amplitude integrals. We will follow this in our applications.

Finally, we note that the separation of the elastic scattering amplitude into three parts, as we have done in (4.14) and (4.19), would be very convenient in determining the role of V_{00} and the φ channel separately. Apparently, this is not possible with the Glauber approximation as outlined in Appendix B, for example.

V. DISCUSSION

The approach to medium-energy-scattering by composite target has been discussed here as a two-step procedure. Firstly, the basis functions φ_t and y_t are obtained along the line discussed in Sec. III, or in some approximations of (2.2) and (2.3). Then, the second step is to construct a set of coupled equations and obtain its solution.

We have thus reduced the complicated many-particle, multichannel scattering problem to a form manageable in practice. Important physical effects known at both low- and high-energy scatterings are incorporated into the theory without regard to their relative importance. The form (2.1) should readily cover the entire range of scattering energies, therefore.

The effect of exchanges and particle transfers may be non-negligible at medium energies, and (2.1) may be immediately generalized to such cases.[17] More detailed forms of φ_t and y_t, and additional simplifications of the coupled equations satisfied by u_0, ω, and χ are more profitably discussed in connection with specific physical applications. A detailed application of the present formalism in the form (4.1), (4.19), and (4.28) to the medium-energy scattering of e^- and e^+ by atomic hydrogen has been carried out and the result will be reported on as a sequel to this paper. Preliminary studies are under way to apply the formalism to the α^-He and p^+H systems.

Notes added in proof. It has been shown recently[21] that the present formulation, in particular Eq. (4.1) with (3.7), is closely related to the optical potential approach of Feshbach and Hüfner[6] and also to the multiple diffraction theory of Glauber.[12] Simple procedures to systematically obtain corrections to the amplitudes calculated by these latter approaches have been developed.[21]

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APPENDIX A

We have emphasized in Secs. II and III that the Eqs. (2.3) and (3.9) for y_t are by no means unique. For high-energy scatterings, other possibilities are available, and we consider a simple case here. If we write the total scattering function as

$$\Psi = P\Psi + Q\Psi \approx \varphi_0 u_0 + \chi y, \tag{A1}$$

then, using the expansion (3.11), we have

$$Q\Psi = G^Q QVP\Psi \approx g_0 QVP\Psi^P \approx g_0 QVP\Phi_i, \tag{A2}$$

where

$$\Phi_i = \psi_0(\vec{r}) e^{i\vec{K}_0\cdot\vec{R}}.$$

(A2) is certainly consistent with the first-order perturbation theory and closely related to the

low-energy analogy of (2.2) and (3.5). Writing (A2) out explicitly as

$$Q\Psi \approx \int g_0(\vec{R}, \vec{R}')(V - \langle V\rangle_{\vec{r}})\psi_0(\vec{r})e^{i\vec{K}_0\cdot\vec{R}'}d\vec{R}', \quad \text{(A3)}$$

and comparing with (A1), we may identify immediately

$$\tilde{y}(\vec{R}, \vec{r})\tilde{\chi} \approx Q\Psi . \quad \text{(A4)}$$

Thus we expect that χ will be close to ψ_0. The main *difference* between (A4) and (3.9) is in the subtraction terms, $\langle V\rangle_{\vec{r}}$ and $\langle V\rangle_{\vec{R}}$, respectively. The resulting χ and u_0 in the two cases will differ markedly. From a physical point of view, (A4) clearly separates out the incoherent part of the scattering and thus gives a more direct connection to the effective-potential treatments such as that given in Refs. 6 and 7. On the other hand, (3.9) follows more readily from the Glauber-type approximation in which the coherent and incoherent components are mixed in Ψ, but the impulse picture stands out.

We also note that (A3) is closely related to the form of $\varphi_t\omega$ of (3.7) obtained in the closure approximation. This suggests that the simple form (2.14a), combined with (3.7), may be quite effective in describing the medium-energy scattering, inspite of the fact that φ_t is essentially a low-energy component of the total wave function. In a similar way, we can approximate (A3) further by introducing the closure approximation as

$$Q\Psi \approx \hat{y}(\vec{R}, \vec{r})\chi(\vec{r}) , \quad \text{(A5)}$$

where

$$\hat{y}(\vec{R}, \vec{r}) = (V - \langle V\rangle_{\vec{r}})e^{i\vec{K}_0\cdot\vec{R}} . \quad \text{(A6)}$$

In (A5), the average energy involved has already been absorbed in $\chi(\vec{r})$, which is yet to be determined from the coupled equations. Obviously, the form (A6) is simpler and more closely related to (3.7) than (A3). On the other hand, (A3) with g_0^{eik} suggests another form for y, as

$$y \approx e^{i\vec{K}_0\cdot\vec{R}}\left[\exp\left(-\frac{i}{K_0}\int_{-\infty}^{z}(V - V_{00})dz'\right) - 1\right] . \quad \text{(A7)}$$

APPENDIX B

The coupled-equation approach to medium-energy scattering, as formulated in Secs. II and III, is designed to improve on the simple Glauber theory for the high-energy small-angle scatterings. We consider here an alternate perturbative procedure, which also clarifies the contents of the Glauber approximation. Thus, possible improvements on the approximate wave function Ψ_G given by (1.10) requires essentially two types of corrections; firstly, it was assumed that

$$T\Phi_G \approx 0 , \quad \text{(B1)}$$

which becomes the more important source of error at large momentum transfer. Certainly, this problem can be treated by an improved method of solution of the coupled equations of Sec. II, taking into account the double and higher multiple *hard* collisions. A simple procedure using the Green's functions in the semiclassical approximation has been considered recently. The second correction to Ψ_G has to do with the way (1.10) incorporates the virtual excitation effect, i.e., the Q-space effect. It is clear that Ψ_G contains a large portion of the $Q\Psi$ through the use of the unprojected potential $V(r, R)$, just as with (3.7) and (A3), but the precise amount included has never been estimated. In the following, we present a simple discussion of Ψ_G and derive a leading correction to the Glauber amplitude, still assuming (B1).

From (1.1) and (2.7a), we have

$$(T + V - E_0')\Psi_i = -B_T\Psi_i , \quad \text{(B2)}$$

where

$$B_T \equiv H_T - E_0 = Q(H_T - E_0)Q . \quad \text{(B3)}$$

The subscript i denotes the initial state of the system. The homogeneous solution of (B2) with the quasielastic boundary conditions and (B1) is given precisely by Ψ_G, as[22]

$$\Psi_{Gi} = \psi_0(\vec{r})e^{i\vec{K}_0\cdot\vec{R}}\Phi_G \quad \text{(B4)}$$

and

$$(T + V - E_0')\Psi_{Gi} \cong 0 . \quad \text{(B5)}$$

Formally, we can then write the solution

$$\Psi_i = \Psi_{Gi} + GB_T\Psi_{Gi} , \quad \text{(B6)}$$

where

$$G = (E + i\epsilon - H)^{-1} . \quad \text{(B7)}$$

The elastic amplitude is given by the two-potential formula as

$$\begin{aligned} \mathcal{T}_{el} &= (\Phi_f, V\Psi_{Gi}) + (\Psi_{Gf}, B_T\Psi) \\ &= (\Phi_f, V\Psi_{Gi}) + (\Psi_{Gf}, B_T\Psi_{Gi}) \\ &\quad + (\Psi_{Gf}, B_T G B_T\Psi_{Gi}) , \end{aligned} \quad \text{(B8)}$$

where

$$\Phi_f = \psi_0(\vec{r})e^{i\vec{K}_f\cdot\vec{R}} .$$

The first term in (B8) is the usual Glauber amplitude

$$\mathcal{T}_{el}^{G} = (\Phi_f, V\Psi_{Gi}) , \quad \text{(B9)}$$

while the leading correction term is given by the second term

$$\mathcal{T}_{el}^{B_T} = (\Psi_{Gf}, B_T \Psi_{Gi}) . \tag{B10}$$

In (B10), Ψ_{Gf} satisfies the same equation (B5) for Ψ_{Gi}, and assumes the form similar to (B4). This is the desired result. Note that the operator B_T in (B10) acts essentially like a potential, because of the property (B3). Thus, $(H_T - E_0)\Psi_{Gi}$ decays for large R like the potential V, so that the integrals involved in (B10) are finite. In the case of Coulomb interactions, as in the electron-atom collisions, V is singular at $\vec{r}_j = \vec{R}$, and H_T acting on Φ_G may introduce unphysical singularities in (B10). However, we expect that the dominant physical contribution to (B10) should come from the region of large $\vec{r}_j$ and small $\vec{R}$. Thus, such singularities are not important in so far as the estimate of $\mathcal{T}_{el}^{B_T}$ is concerned; we may avoid such singularities by, for example, introducing a cut-off in V which appears in Φ_G, as

$$V = -\frac{z_c e^2}{R} + \sum_j \frac{e^2}{|\vec{r}_j - \vec{R}|} \to -\frac{z_c e^2}{R+a} + \sum_j \frac{e^2}{|\vec{r}_j - \vec{R}| + a} \quad (a \gtrsim 0) . \tag{B11}$$

Other ways of dealing with this problem are also possible.[23] The modifications such as (B11) may sometimes also be required for φ of (3.7) and $\hat{y}$ of (A6).

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