Distorted - wave theory of multistep processes^{*}

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Robson's criticism of the distorted-wave's Green's function, used for intermediate states in higher-order calculations, is examined and shown to be unfounded. Possible difficulties of his suggested alternative method for higher-order calculations are considered.

In a paper with the above title¹ Robson discusses difficulties that may appear if the distorted-waves formulation of reaction theory is carried to second-order Born approximation. Standard calculations that use the Green's function for a complex potential (method A of Ref. 1) are felt to suffer from spurious creation of flux in intermediate states. A new approach (method B) is therefore proposed, based on the multichannel expansion of the exact many-body Green's function. We show here that the usual method A Green's function does not encounter difficulty due to creation of flux in intermediate states; this weakens the motivation for complicated new approaches such as method B. We show further that method B is subject to criticism for double counting of intermediate states.

This is not to say that usual higher-order distorted-wave Born approximation (DWBA) has no problems at all. Various formulations of the Born series are known to diverge, particularly if rearrangement boundary conditions are allowed to play a role; this might be relevant if many terms in the series could be computed. Moreover, we recognize² that direct reaction theories in principle use *effective operators* (such as optical potentials) defined in a very restricted portion of Hilbert space. Great care is required to include effective operators consistently in higher-order analyses. Fortunately, neither of these questions is at issue in the present discussion.

Robson's article¹ discusses the "multiple" DWBA amplitude

$$\hat{T}^{(M)}_{\beta\alpha} = \langle \chi^{(-)}_{\beta} | \hat{V}_{\beta} G^{(+)} \hat{V}_{\alpha} | \chi^{(+)}_{\alpha} \rangle \quad , \tag{1}$$

in which $\chi_{\alpha}^{(+)}$ and $\chi_{\beta}^{(-)}$ are distorted waves defined in channels α and β , \hat{V}_{α} and \hat{V}_{β} are residual interactions defined with respect to those channels, and

$$G^{(+)} = (E + i\epsilon - H)^{-1}$$
(2)

is the exact Green's function for the many-body scattering system. At issue is the choice of approximations to $G^{(+)}$. Two methods are contrasted:

(A) $G^{(+)}$ is expanded in a distorted-waves Born series, through a chain of essentially arbitrary intermediate arrangements. The series is truncated at second order, giving an approximation, $G^{(+)} \approx G_A^{(+)}$, defined with respect to one particular intermediate arrangement. (B) $G^{(+)}$ is expanded in an exact bilinear series of eigenfunctions of H, and heuristically motivated distorted-waves approximations of the intermediate eigenfunctions are inserted in this series. Thus method A discusses $G^{(+)}$ in terms of a particular intermediate arrangement, whereas method B sums over all possible intermediate arrangements. Method B is suggested because of supposed difficulties of method A.

In either method, bilinear expansions of $G^{(+)}$ allow Eq. (1) to be put in the form of a sum of products of off shell *T*-matrix amplitudes,¹ provided suitable transformations with the *S* matrix are introduced. We do not emphasize these transformations, because they are not central to the problem of approximating the multiple amplitude. We mainly treat the questions of how to reduce Eq. (1) for practical calculation, what are the properties of Eq. (1) in the presence of strong absorption, how the alternative reductions of Eq. (1) compare.

Method A is most clearly discussed for a single intermediate channel γ , which may have an arrangement different from that of either channel α or channel β . The eigenfunctions defined in the intermediate channel are

$$\phi_{\gamma}(\xi)\chi^{(+)}(\vec{\mathbf{k}},\vec{\mathbf{r}}) , \qquad (3)$$

in which $\phi_{\gamma}(\xi)$ is the internal wave function that defines channel γ , and $\chi^{(+)}(\vec{k}, \vec{r})$ are distorted waves for the scattering of the fragments in channel γ , with \vec{k} the asymptotic relative momentum of the fragments and \vec{r} their displacement from each other. Use of these eigenfunctions to construct a bilinear expression for the Green's function requires integration over all values of \vec{k} .

The wave functions $\chi^{(+)}(\vec{k}, \vec{r})$ are governed by a non-Hermitian optical potential $U_{\gamma}(\vec{r})$; as a result distorted waves for different $|\vec{k}|$ values are not orthogonal. This nonorthogonality must be dealt

10

2623

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with when the Green's function is constructed. The usual procedure is to extend the set $\chi^{(+)}(\vec{k}, \vec{r})$ into a biorthogonal set by introducing wave functions dual to the distorted waves.

The properties of the dual set of wave functions and the structure of the distorted-waves Green's function are most easily seen³ in partial-wave expansion. Let us discuss only the *s*-wave term of $\chi^{(+)}(\vec{k}, \vec{r})$,

$$\chi^{(+)}(\vec{k},\vec{r}) - \frac{f(k,r)}{kr}$$
, (4)

in which f(k, r) is the radial wave function that reduces outside the potential $U_{\gamma}(r)$ to the expression

$$f(k,r)_{\text{outside}} = \frac{i}{2} \left[e^{-ikr} - \eta(k) e^{ikr} \right] \quad , \tag{5}$$

with incoming flux of standard magnitude. Then the f(k, r) are found to be self-dual, *provided complex conjugation is not used* in scalar products. The scalar product of f(k, r) with itself is found to be proportional to the reflection coefficient $\eta(k)$. Use of these properties immediately gives the l=0 radial distorted-waves Green's function³

$$G_{A}^{(+)}(r,r')_{l=0} = \left(\frac{2}{\pi}\right) \int_{0}^{\infty} dk \, \frac{f(k,r)f(k,r')}{\eta(k)(E_{\gamma} + i\epsilon - \hbar^{2}k^{2}/2\mu)} \,.$$
(6)

We note again the omission of complex conjugation. [In principle a few bound state terms may have to be added in Eq. (6). These do not affect qualitative discussions.] The normalization factor $\eta(k)$ in the denominator is intriguing, because

substitute Eq. (5) into Eq. (6), to get

if the optical potential is strongly absorbing we can have

$$|\eta(k)| \ll 1 \quad . \tag{7}$$

Robson suggests that small η can cause a "creativity problem", resulting in undesirable enhancement of the multistep amplitude.

Equation (7) certainly indicates the need for great care in the application of Eq. (6) in practical calculations. However, the actual somewhat secondary role of the factor $\eta(k)$ is at once indicated by going over to the well-known, exact closed form of the outgoing-wave Green's function

$$G_{A}^{(+)}(\boldsymbol{r},\boldsymbol{r}')_{l=0} = \left(\frac{2\mu}{\hbar^{2}k}\right) f(\boldsymbol{k},\boldsymbol{r}_{<})h(\boldsymbol{k},\boldsymbol{r}_{>}) \quad , \tag{8}$$

where $r_{<}$, $r_{>}$ indicate the lesser and greater of r, r' and h(k, r) is the irregular optical-model radial wave function that reduces outside the potential $U_{\gamma}(r)$ to the normalized exponential

$$h(k,r)_{\text{outside}} = e^{ikr} \quad . \tag{9}$$

The closed form Green's function of Eq. (8) is manifestly well behaved in the limit $\eta(k) \rightarrow 0$. Therefore the apparent "creativity problem" in Eq. (6) is an artifact of the bilinear expansion.

Although Eqs. (6) and (8) are by construction identical solutions of the same differential equation, it is instructive to insert explicit wave functions in Eq. (6) and discuss the integrations to see qualitatively, how the apparent creativity problem of the bilinear expansion is overcome when the closed form is recovered. If we work in the region r, r' external to the potential $U_{r}(r)$, we may

$$G_{A}^{(+)}(r,r')_{l=0} = \frac{1}{2\pi} \int_{0}^{\infty} dk \, \frac{e^{ik(r-r')} + e^{ik(r'-r)} - \eta e^{ik(r+r')} - \eta^{-1} e^{-ik(r+r')}}{(E_{\gamma} + i\epsilon - \hbar^{2}k^{2}/2\mu)} \,. \tag{10}$$

Equation (10) is easy to discuss as a contour integral if $\eta(k)$ is treated as constant. The first three terms give pole contributions, which precisely yield Eq. (8) for the external region. The third term also gives an integral along the imaginary k axis, and the fourth term, the problematic term proportional to η^{-1} , gives only an integral of this type. Because (r+r')>0, the imaginary integrals tend to be small. They vanish in the limit that r or r'becomes asymptotically large. This effect is already visible in Eq. (10), where the η^{-1} term is seen to contain a rapidly oscillatory phase factor. which reduces its contribution when the k integration is performed, as in previous discussions of phase averaging.²⁻⁴ To complete the analysis of Eq. (10) it would be necessary to take the k dependence of $\eta(k)$ into account, at least to the extent of

specifying its analytic properties. However these further steps are of no present interest, because the exact answer is already in hand.

The limited role of absorptivity is most easily realized by considering $G_A(r, r')$ at r = r'. The Green's function is a solution of a differential equation that contains a localized source; near this source the properties of the solution are dominated by the source, not by absorptivity in the propagator. Therefore $G_A(r', r')$ cannot have any over-all dependence on η . For $r \neq r'$ the smaller argument in Eq. (8), the one that lies deeper in the optical potential, always appears in the regular function $f(k, r_{<})$, the function that is *reduced* by absorption. No matter to what extent creativity might cause $h(k, r_{>})$ to grow, this irregular function is multiplied by $f(k, r_{<})$, and the product is not greater than at r = r'. In other words, the net effect of propagation in intermediate states from r' to r is loss of probability amplitude, not creation. The intermediate Green's function must be seen as a whole, not factor by factor.

Since small η does not cause G_A to be unusually large, it does not matter with what other factors G_A is associated in Eq. (1), contrary to remarks at the end of Sec. II of Ref. 1. Therefore there is no reason to fear that other details of this amplitude might enhance the role of "creativity".

To develop method B we construct an exact bilinear expansion of $G^{(+)}$ in Eq. (1), using multichannel scattering eigenfunctions $\Psi_{\lambda}^{(+)}$ of the complete H,

$$H\Psi_{\lambda}^{(+)} = E_{\lambda}\Psi_{\lambda}^{(+)} \quad . \tag{11}$$

Different eigenfunctions $\Psi_{\lambda}^{(+)}$ are distinguished by their total energy E_{λ} , and by the arrangement rand channel ρ in which they have ingoing waves. Hence $\{\lambda\} \equiv \{E_{\lambda}, r, \rho\}$. Eigenfunctions that differ in any of these indices are orthogonal.⁵ The exact Green's function takes the form

$$G^{(+)} = \sum_{\lambda} \frac{|\Psi_{\lambda}^{(+)}\rangle\langle\Psi_{\lambda}^{(+)}|}{E + i\epsilon - E_{\lambda}} \quad .$$
 (12)

Again, completeness may require adding a few bound-state terms to this expression.

Robson now seeks approximations to Eq. (12), not by truncating the sum, but by devising distorted-waves replacements for the state vectors. Because insertion of Eq. (12) in Eq. (1) does not give an expression composed of *T*-matrix elements, he doesn't simply substitute distorted waves in Eq. (12) as it stands. The bra vectors are instead replaced with corresponding time-reversed eigenvectors, by use of the scattering matrix, so that

$$G^{(+)} = \int dE' \sum_{\substack{r,\rho \\ t\tau}} \frac{|\Psi_{E'r\rho}^{(+)} S_{r\rho,t\tau}^{\dagger} \langle \Psi_{E't\tau}^{(-)} |}{E + i\epsilon - E'} .$$
(13)

The eigenvectors and the S matrix in Eq. (13) are all computed at the same energy E', which we have made explicit.

Method B consists¹ in introducing optical approximations in Eq. (13). The optical S matrix is assumed identical to the exact S matrix, under the restriction t = r. The ket is replaced by the generalized distorted wave $\chi_{E'r\rho}^{(+)}$ that is ingoing in channel ρ and can scatter inelastically to other channels in $r, \rho' \neq \rho$. The bra is replaced by the corresponding dual vector $\chi_{E'r\tau}^{(-)}$. The approximate Green's function then is

$$G_{B}^{(+)} = \int dE' \sum_{r,\rho\rho''} \frac{|\chi_{E'r\rho}^{(+)} \rangle S_{r\rho,r\rho''}^{\dagger} \langle \chi_{E'r\rho''}^{(-)}|}{E + i\epsilon - E'} \quad .$$
(14)

This result seems more symmetrical than if corresponding optical approximations had been used directly in Eq. (12). Insertion of Eq. (14) in Eq. (1) gives an expression composed of products of DWBA amplitudes (or coupled-channel Born approximation, to be precise) summed over a large array of intermediate energies, arrangements, and channels.

The significance of method B must be judged in the light of our previous demonstration that method A leads to perfectly finite results for the multistep amplitude, even for the strong absorption limit $\eta \neq 0$. It is not necessary to devise new approaches to overcome a divergence of method A. Therefore method B is not so much a possible solution of a key problem of multistep calculations, but rather is one of several alternative definitions of the multistep DWBA amplitude. On the other hand, method B uses a lengthy expansion in a potentially dangerous set of intermediate states: although the exact multichannel wave functions in Eq. (12) are orthogonal and can meaningfully be summed over arrangements, this orthogonality is destroyed when optical approximations are introduced. The summation in Eq. (14) thus involves considerable overcounting, as a result of the overlaps between different arrangements in the nuclear interior. No such overcounting occurs in method A, which is based on a single intermediate arrangement and expands only in the (orthogonal) states of excitation of the nuclei in that arrangement. The more extensive sum in $G_B^{(+)}$ is therefore very likely to outweigh any tendency for the individual terms in $G_B^{(+)}$ to be smaller than those in $G_{A}^{(+)}$. Comparison with experiment certainly cannot decide which of these mathematical approximations should be preferred. Perhaps, then, ambitious applications of method B should be deferred until a more complete analysis is available.

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