Nonorthogonality Effects in Successive Particle-Transfer Reactions

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It is demonstrated that nonorthogonality effects can play a very important role in multistep processes involving successive particle-transfer reactions. This is shown for the particular example of the $(^3\mathrm{He},d)$-(d,t) process, where nonorthogonality terms can be included as a renormalization of the effective interaction for the direct $(^3\mathrm{He},t)$ charge-exchange process.

Recently, the importance of successive one-particle pickup-stripping (^{3}He-α-t) processes in $(^3\mathrm{He},t)$ reactions has been demonstrated by several authors.[1-5] These calculations, based on the second-order distorted-wave Born approximation (DWBA), showed that inclusion of the ^{3}He-α-t and ^{3}He-d-t processes can explain many observed anomalies in $(^3\mathrm{He},t)$ cross sections which defy explanation in terms of the single-step, direct charge-exchange mechanism.

All the calculations done so far, however, neglect the so-called nonorthogonality correction,[6-11] which arises because inner products of basis state functions describing different mass partitions do not vanish. The aim of the present work is to propose a method to deal with this basis nonorthogonality in the coupled-reaction-channels (CRC) formalism[4] and to discuss its consequences, taking as an example the $(^3\mathrm{He},t)$ reaction. We shall show that the effects of nonorthogonality can be very large.

Here, we closely follow Ref. 4, where the CRC equations were obtained neglecting nonorthogonality effects. In order to take into account these effects we are led to distinguish between two types of CRC distorted wave functions, $\chi_\alpha(\vec{r}_\alpha)$ and $X_\alpha(\vec{r}_\alpha)$, defined respectively as

$$\chi_\alpha(\vec{r}_\alpha) \equiv (\alpha|\Psi\rangle , \tag{1}$$

$$|\Psi\rangle \equiv \sum_\alpha X_\alpha(\vec{r}_\alpha)|\alpha\rangle , \tag{2}$$

where $|\Psi\rangle$ is the total state function of the system and $|\alpha\rangle$ is the channel basis function, describing the intrinsic state of the projectile a and nucleus A. Thus $|\alpha\rangle \equiv |aA\rangle \equiv \psi_a(\xi_a)\psi_A(\xi_A)$, where ξ_a and ξ_A are the sets of internal coordinates of systems a and A, respectively. We shall consistently use the notation $(\alpha|\rangle$ to mean that only an internal coordinate integration has been performed, with the channel radius $\vec{r}_\alpha$ being held fixed, i.e.,

$$(\alpha|\,\varphi\rangle \equiv \langle\alpha|\,\varphi\rangle|_{\vec{r}_\alpha}. \tag{3}$$

In principle, the full set of basis states $|\alpha\rangle$ is overcomplete. If all the bound and continuum states for one mass partition were included, then the states of all other mass partitions could be expanded in terms of that one set. In practice, however, one must represent the total state function with as few terms as possible, and thus always the basis is drastically truncated. The scheme of the CRC approach is, then, that a description in terms of a few states of different mass partitions of the system gives a much more useful representation of the total system state than an expansion in terms of a vast number of states of a single mass partition. At the same time, problems of overcompleteness are avoided by the drastic truncation.

Because of the nonorthogonality of the different basis functions $|\alpha\rangle$, the distorted waves χ_α and X_α cannot be assumed to be identical, except in the asymptotic region. They are connected through the relations (1) and (2); indeed, if Eq. (2) is inserted into (1) we obtain

$$\chi_\alpha(\vec{r}_\alpha) = \sum_\beta (\alpha|X_\beta(\vec{r}_\beta)|\beta\rangle = \sum_\beta \int d^3r_\beta (\alpha|\beta) X_\beta(\vec{r}_\beta), \tag{4}$$

where in the overlap integral $(\alpha|\beta)$ both channel radii are held fixed. That is, the integration is over the particular set of internal coordinates common to both channels, ξ_i, only. Specifically,

$$\{\vec{r}_\alpha, \xi_\alpha\} = \{\vec{r}_\beta, \xi_\beta\} = \{\vec{r}_\alpha, \vec{r}_\beta, \xi_i\}. \tag{5}$$

We define the nonorthogonality function $N_{\alpha\beta}(\vec{r}_\alpha, \vec{r}_\beta)$ by

$$(\alpha|\beta) = \delta_{\alpha,\beta}\delta(\vec{r}_\alpha - \vec{r}_\beta) + N_{\alpha\beta}(\vec{r}_\alpha, \vec{r}_\beta), \tag{6}$$

so that Eq. (4) may be rewritten as

$$X_\alpha(\vec{r}_\alpha) = \chi_\alpha(\vec{r}_\alpha) - \sum_\beta \int d^3r_\beta\, N_{\alpha\beta}(\vec{r}_\alpha, \vec{r}_\beta) X_\beta(\vec{r}_\beta). \tag{7}$$

With this relation, we can solve for X in terms of χ formally or numerically, for instance by an iterative method.

It is now straightforward to establish the coupled-reaction-channel equations for the functions χ. Inserting Eq. (2) into the full Schrödinger equation,

$$(T_\alpha + U_\alpha - E_\alpha)(\alpha|\Psi\rangle = -(\alpha|V_\alpha - U_\alpha|\Psi\rangle, \tag{8}$$

we get, making use of Eq. (7),

$$(T_\alpha + U_\alpha - E_\alpha)\chi_\alpha(\vec{r}_\alpha) = -\sum_\beta \int d^3r_\beta (\alpha|V_\alpha - U_\alpha|\beta)\chi_\beta(\vec{r}_\beta) + \sum_{\beta,\gamma} \int d^3r_\beta d^3r_\gamma\, (\alpha|V_\alpha - U_\alpha|\beta) N_{\beta\gamma}(\vec{r}_\beta, \vec{r}_\gamma) X_\gamma(\vec{r}_\gamma). \tag{9}$$

These are the CRC equations as obtained in Ref. 4, with an additional term on the right-hand side (rhs) which arises from nonorthogonality.

In order to understand the effect of the additional terms in Eq. (9), let us use the second-order DWBA, which has been shown to be a good approximation to the amplitude given by the full CRC equations for the pickup-stripping process $(^3\mathrm{He}, \alpha)$-(α, t).[4] The transition amplitude for (α, β) is generally obtained by solving an inhomogeneous equation for the final channel β, which we write explicitly as

$$(T_\beta + U_\beta - E_\beta)\chi_\beta(\vec{r}_\beta) = -\int d^3r_\alpha (\beta|\overline{V}_\beta|\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha) + \int d^3r_\gamma d^3r_\gamma' d^3r_\alpha \sum_\gamma (\beta|\overline{V}_\beta|\gamma) G_\gamma(\vec{r}_\gamma, \vec{r}_\gamma')(\gamma|\overline{V}_\gamma|\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha) + \int d^3r_\gamma d^3r_\alpha \sum_\gamma (\beta|\overline{V}_\beta|\gamma) N_{\gamma\alpha}(\vec{r}_\gamma, \vec{r}_\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha). \tag{10}$$

Here, $G_\gamma(\vec{r}_\gamma, \vec{r}_\gamma')$ is the optical-model Green's function for the intermediate projectile, and $\chi_\alpha^{(0)}(\vec{r}_\alpha)$ is the entrance-channel distorted wave, obtained from the optical-model Schrödinger equation, $(T_\alpha + U_\alpha - E_\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha) = 0$. Finally, $\overline{V}_\beta$ and $\overline{V}_\gamma$ are the effective-interaction potentials associated with the direct (α, β) reaction and the (γ, β) [or (α, γ)] stripping (or pickup) process. In deriving Eq. (10) we have consistently retained terms only up to second order. Thus, we replaced X_α by χ_α in the third term on the rhs, which is the only new term. The first term on the rhs describes the direct (α, β) process, while the second gives the second-order (α, γ)-(γ, β) contribution,[1-5] obtained by taking $\beta = \gamma$ on the rhs of Eq. (9) and using

$$(T_\gamma + U_\gamma - E_\gamma)\chi_\gamma(\vec{r}_\gamma) = -\int d^3r_\alpha (\gamma|\overline{V}_\gamma|\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha). \tag{11}$$

The transition amplitude for (α, β) obtained from (10) can be written as

$$T_{\beta\alpha} = T_{\beta\alpha}^{(1)} + T_{\beta\alpha}^{(2)} + T_{\beta\alpha}^{(\mathrm{no})}, \tag{12}$$

where

$$T_{\beta\alpha}^{(1)} = \int d^3r_\beta d^3r_\alpha\, \chi_\beta^{(0)}(\vec{r}_\beta)(\beta|\overline{V}_\beta|\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha), \tag{13a}$$

$$T_{\beta\alpha}^{(2)} = -\int d^3r_\beta d^3r_\gamma d^3r_\gamma' d^3r_\alpha \sum_\gamma \chi_\beta^{(0)}(\vec{r}_\beta)(\beta|\overline{V}_\beta|\gamma) G_\gamma(\vec{r}_\gamma, \vec{r}_\gamma')(\gamma|\overline{V}_\gamma|\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha), \tag{13b}$$

$$T_{\beta\alpha}^{(\mathrm{no})} = -\int d^3r_\beta d^3r_\gamma d^3r_\alpha \sum_\gamma \chi_\beta^{(0)}(\vec{r}_\beta)(\beta|\overline{V}_\beta|\gamma) N_{\gamma\alpha}(\vec{r}_\gamma, \vec{r}_\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha). \tag{13c}$$

$T_{\beta\alpha}^{(1)}$, $T_{\beta\alpha}^{(2)}$, and $T_{\beta\alpha}^{(\mathrm{no})}$ are the contributions coming from the first and second DWBA and the nonorthogonality correction, respectively.

An important remark which should be made at this stage is that the explicit form of $T_{\beta\alpha}^{(\mathrm{no})}$ will depend on whether one chooses the post or the prior form for the interaction matrix elements in $T_{\beta\alpha}^{(2)}$.[12] Thus, for instance, if one uses the prior-post form for the $(^3\mathrm{He}, \alpha)$-(α, t) process, instead of the post-post form occuring in Eq. (13b), the nonorthogonality correction actually vanishes; i.e., the term given by (13c) is formally canceled by a term that appears when the transformation is made from the post-post to the required prior-post form.[12]

Summarizing the resultant nonorthogonality term for the four possible choices of the effective inter-

action potentials, we get

$$T_{\beta\alpha}^{(\mathrm{no})} = 0 \text{ (prior-post)}, \tag{14a}$$

$$T_{\beta\alpha}^{(\mathrm{no})} = -\sum_\gamma \int d^3r_\beta d^3r_\gamma d^3r_\alpha \chi_\beta^{(0)}(\vec{r}_\beta) N_{\beta\gamma}(\vec{r}_\beta, \vec{r}_\gamma)(\gamma|V_\alpha|\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha) \text{ (prior-prior)}, \tag{14b}$$

$$T_{\beta\alpha}^{(\mathrm{no})} = -\sum_\gamma \int d^3r_\beta d^3r_\gamma d^3r_\alpha \chi_\beta^{(0)}(\vec{r}_\beta)(\beta|V_\gamma|\gamma)N_{\gamma\alpha}(\vec{r}_\gamma, \vec{r}_\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha)$$
$$-\sum_\gamma \int d^3r_\beta d^3r_\gamma d^3r_\alpha \chi_\beta^{(0)}(\vec{r}_\beta) N_{\beta\gamma}(\vec{r}_\beta, \vec{r}_\gamma)(\gamma|V_\alpha|\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha) \text{ (post-prior)}, \tag{14c}$$

$$T_{\beta\alpha}^{(\mathrm{no})} = -\sum_\gamma \int d^3r_\beta d^3r_\gamma d^3r_\alpha \chi_\beta^{(0)}(\vec{r}_\beta)(\beta|V_\beta|\gamma)N_{\gamma\alpha}(\vec{r}_\gamma, \vec{r}_\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha) \text{ (post-post)}. \tag{14d}$$

As is well known, practically speaking it is always necessary to use the post form in calculating the stripping process, while the prior form is necessary for the pickup process. Hence, for the calculation of a two-step process such as $(^3\mathrm{He},\alpha)$-(α,t), we have to use the prior-post form. Thus, we have no nonorthogonality correction term. However, if we also include the $(^3\mathrm{He},d)$-(d,t) process,[3,5] we must use the post-prior form and pay the penalty of *two* nonorthogonality correction terms!

To study the importance of these nonorthogonality corrections, we made a simple estimate of the terms in Eq. (14c), based on the zero-range approximation for the overlap integrals involving light projectile wave functions. We consider the $(^3\mathrm{He},d)$-(d,t) process as an example.[3,5] Using the approximations we have enumerated, and noticing that in any realistic calculation[1-5] all of the intermediate nuclear states C which can be reached from the target ground state A and which lead to the specific nuclear state B are in fact included, the nonorthogonality term can be put into the same form as the direct term, with a δ-function interaction potential. Thus, for instance, the first term of Eq. (14c) is written as

$$-\int d^3r_\beta d^3r_\alpha \chi_\beta^{(0)}(\vec{r}_\beta)(\beta|V_{\mathrm{no}}|\alpha)\chi_\alpha^{(0)}(\vec{r}_\alpha)\delta(\vec{r}_\alpha - \vec{r}_\beta), \tag{15}$$

where

$$V_{\mathrm{no}} = \sum_i \sum_s a_{s1}\delta(\vec{r}_\alpha - \vec{r}_i)(\hat{\sigma}_s^{(\alpha)}\cdot\hat{\sigma}_s^{(i)})(\hat{\tau}^{(\alpha)}\cdot\hat{\tau}^{(i)}), \tag{16}$$

with i denoting the ith nucleon in the target nucleus A and

$$a_{s1} = (-)^s\{3/[8(2s+1)]\}D_0\Delta_0. \tag{17}$$

Also $\hat{\sigma}_s$ is either the unit operator or the spin operator, for $s=0$ or 1, respectively, and $\hat{\tau}$ is the corresponding isospin operator. D_0 and Δ_0 are the zero-range constants given by

$$D_0 = \int d^3r \int d^3\rho\, \varphi_d(\rho)V_{dt}\varphi_t(r,\rho)$$

and

$$\Delta_0 = \int d^3r \int d^3\rho\, \varphi_d(\rho)\varphi_t(r,\rho),$$

φ_t and φ_d being the triton and deuteron internal wave functions, respectively. If use is made of the values $D_0 = -183.6$ MeV fm$^{3/2}$ and $\Delta_0 = 29.3$ fm$^{3/2}$ obtained by Bassel,[13] we get $a_{10} = -2020$ MeV fm^3 for $s=0$, implying that the resultant effective interaction arising from nonorthogonality is attractive, in contrast to the repulsive interaction for the direct, charge-exchange process.

The second term of Eq. (14c) can be estimated in a similar way. Note, however, that the interaction matrix element is given in the prior form instead of the post form ordinarily adopted for calculating the $(^3\mathrm{He},d)$ process. Nevertheless, one can estimate the term using the zero-range approximation introduced before, and the result can be given in the same form as Eqs. (15)–(17) with the following two modifications: $\delta(\vec{r}_\alpha - \vec{r}_i) \to \delta(\vec{r}_\alpha - \vec{r}_i)V(\vec{r}_i)$, where $V(\vec{r})$ is the potential binding the picked-up proton to the target; and $D_0\Delta_0 \to \Delta_0^2$. Even with these modifications, it is difficult to make an estimate of the effective interaction volume of the resulting "direct" amplitude. However, it is clear that the net effective interaction resulting from both these terms is still attractive. Thus, in order to get a rough idea of the importance of the nonorthogonality corrections, one may simply compare the estimate $a_{01} = -2020$ MeV fm^3 with the corresponding values used in the direct $(^3\mathrm{He},t)$ DWBA calculations of the past. With a Yukawa two-body interaction having $V = 20$ MeV and a range parameter of 0.73 fm^{-1}, as suggested by the direct $(^3\mathrm{He},t)$ analysis of Kossanyi-Demay *et al.*,[14] one obtains 640 MeV fm^3. On the other hand, studies of the (p,p') and (p,n) reactions suggest an effective two-nucelon interaction with a volume integral of 125–250 MeV fm^3.[15-18] We are forced to conclude that, even if the estimate of the nonorthogonality contribution is correct only to within an order of magnitude, the nonorthogonality term will in gen-

eral make a very sizable contribution to the (^{3}He, t) amplitude. The general effect would be that, in second-order DWBA or CRC calculations which ignore the nonorthogonality correction, the direct amplitude would need to have the wrong phase relative to the two-step terms in order to fit the data. This phase difficulty has already been noticed in a number of instances.[1,3,4]

Such effects of nonorthogonality are by no means restricted to charge-exchange reactions, but would be expected to manifest themselves in any reaction with a significant multistep contribution. For example, recent calculations for successive nucleon-transfer processes in heavy-ion reactions clearly show the importance of the nonorthogonality contributions.[11,18]

Better estimates of the nonorthogonality contributions to the cases we have discussed require full finite-range treatment of the overlap integrals. Detailed calculations are now underway by the present authors.

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Simple Potential Model for Nucleus-Nucleus Interactions*

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We construct a simple optical potential for nucleus-nucleus processes by a folding method. With these potentials, we have obtained high-quality fits to a variety of elastic-scattering data. We also successfully reproduce one-particle transfer data. However, two-particle transfer results may indicate the need for further refinements of the model. In addition, we calculate the bound states of an $\alpha + {}^{16}$O folded potential. There is good agreement with experimental energies and α widths for two α-cluster bands in ^{20}Ne.

A simple folding model, where the optical potential is given by a convolution of the target density with an effective nucleon-nucleon interaction, is quite successful in the description of nucleon-nucleus elastic scattering.[1] In view of the considerable amount of heavy-ion elastic scattering and transfer data which has recently become available, it seems particularly relevant to study the application of this simple and physically appealing technique to heavy-ion processes. A generalization of this model to nucleus-nucleus interactions yields an optical potential of the form

$$V_{\rm opt}(\vec{r}) = -\frac{2\pi\hbar^2\bar{f}}{M}\int d^3r'\,\rho_1(\vec{r}'-\vec{r})\rho_2(\vec{r}'). \qquad (1)$$

In Eq. (1), ρ_1 and ρ_2 are the projectile and target total densities, respectively, M is the nucleon