Heavy-ion distorted-wave Born-approximation recoil to second order in a Taylor series*

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The perturbative approach for rapid calculation of recoil corrections to the heavy-ion distorted-wave Born approximation has been extended to second order without further approximation. The resulting calculational scheme turns out to be so well converged as to be essentially exact finite range for single nucleon transfer at energies not too far above the Coulomb barrier.

[NUCLEAR REACTIONS Proper second order recoil DWBA. ^{48}Ca(^{14}N, ^{13}C) $E=50$; Q and α (scaling parameter) dependence of calculated σ.]

I. INTRODUCTION

The continuing interest in heavy-ion induced reactions makes still pertinent the problem of performing distorted-wave Born-approximation DWBA calculations as rapidly as is consistent with reasonable accuracy. A proper first order Taylor series expansion in the recoil parameter has been previously described.[1] The present paper describes the extension of the proper Taylor series approach to the exact calculation of quadratic recoil effects.[2] Comparison with "in principle" exact DWBA calculations has shown that at energies not too far above the Coulomb barrier, single nucleon transfer calculations utilizing the second order Taylor series method are so well converged as to be essentially exact finite range.[3] While the present formalism adds nothing new to the fundamental reaction theory, it does provide the possibility of performing larger numbers of exploratory calculations since the amount of time required per calculation is about $\frac{1}{20}$ of that required for an exact calculation using, for example, LOLA.[4]

II. FORMALISM

In this section the expressions for the second order recoil terms will be worked out in detail. These terms can then be combined with the zeroth order (no recoil)[5] and first order recoil[1] formulas to build a rapid calculational scheme. The notation used will be consistent with Ref. 1, and free reference will be made to that paper to avoid needless repetition.

A single nucleon transfer reaction is considered of the form:

$$(A+N)+B \rightarrow A+(B+N)$$

with $(A+N)$ the projectile and B the target nucleus. If spin orbit interactions are ignored, the DWBA amplitude to be evaluated may be written[1]

$$I^{l_1 l_2 LM} = \sum_{m_1 m_2} \langle l_2 m_2 LM | l_1 m_1 \rangle \langle \psi^{(-)}(\vec{k}_f, \vec{r}_f)\, \varphi_{j_2}^{l_2 m_2}(\vec{r}_2) | V(\vec{r}_1) | \varphi_{j_1}^{l_1 m_1}(\vec{r}_1) \psi^{(+)}(\vec{k}_i, \vec{r}_i) \rangle \ , \tag{1}$$

where $\psi^{(+)}(\vec{k}_i, \vec{r}_i)$, $\psi^{(-)}(\vec{k}_f, \vec{r}_f)$ are the entrance and exit scattering wave functions and $\varphi_{j_1}^{l_1 m_1}$, $\varphi_{j_2}^{l_2 m_2}$ are the wave functions for the transferred particle bound to the projectile or residual nucleus. The coordinate system is illustrated in Fig. 1. The sole approximation to be made in evaluating Eq. (1) is in the argument of $\psi^{(-)}$ which is exactly $\vec{r}_f$.

From the exact relations

$$\vec{r}_f = \beta \vec{r}_i + \gamma \vec{r}_1, \quad \beta = \frac{M_B}{M_B + M_N} \ , \qquad \gamma = \frac{(M_A + M_B + M_N) M_N}{(M_A + M_N)(M_B + M_N)} \tag{2}$$

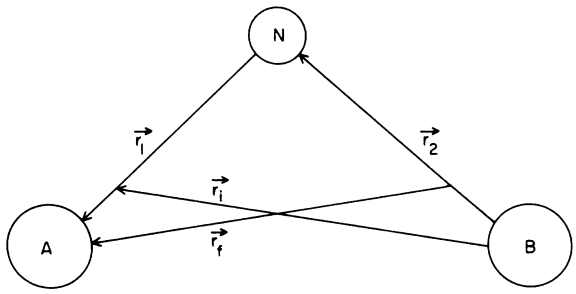

FIG. 1. Coordinate vectors for single nucleon transfer.

one may write $\vec{r}_f$ in terms $\vec{r}_i$, $\vec{r}_1$ and an arbitrary parameter α

$$\vec{r}_f = \alpha\,\vec{r}_i + [\,(\beta-\alpha)\,\vec{r}_i + \gamma\,\vec{r}_1\,]\ . \tag{3}$$

Then $\psi^{(-)}$ may be expanded about $\alpha\,\vec{r}_i$ to second order as

$$\psi^{(-)}(\vec{r}_f) = \psi^{(-)}(\alpha\,\vec{r}_i) + \left(1+\frac{(\beta-\alpha)}{2\alpha}\right)\frac{(\beta-\alpha)}{\alpha}\,r_i\,\frac{\partial\psi^{(-)}}{\partial r_i}(\alpha\,\vec{r}_i) + \left(1+\frac{(\beta-\alpha)}{2\alpha}\right)\frac{\gamma}{\alpha}\,\vec{r}_1\cdot\nabla_i\psi^{(-)}(\alpha\,\vec{r}_i)$$
$$+\frac{(\beta-\alpha)^2}{2\alpha^2}\,r_i^{\,2}\,\frac{\partial^2\psi^{(-)}}{\partial r_i^{\,2}}(\alpha\,\vec{r}_i) + \frac{(\beta-\alpha)\gamma}{\alpha^2}\,r_i\,\vec{r}_1\cdot\nabla_i\,\frac{\partial\psi^{(-)}}{\partial r_i}(\alpha\,\vec{r}_i) + \frac{\gamma^2}{2\alpha^2}\,(\vec{r}_1\cdot\nabla_i)^2\psi^{(-)}(\alpha\,\vec{r}_i) \tag{4}$$

and this result may be inserted into Eq. (1). The first term is the no-recoil term discussed elsewhere.[5,1] The second and third terms comprise the first order recoil components discussed in detail in Ref. 1, with the additional $(\beta-\alpha)/2\alpha$ contributions coming from second order. The fourth term, which vanishes when $\alpha=\beta$, can be calculated by a minor modification of a no-recoil code. The fifth term, which also vanishes when $\alpha=\beta$, can be calculated by a minor modification of the first order code following the formalism of Ref. 1. Thus only the sixth term, corresponding to the fundamental second order recoil effects, will be considered here in detail. Making the explicit substitution into Eq. (1) one obtains

$$I_{(2)}^{l_1 l_2 LM} = \frac{\gamma^2}{2\alpha^2}\sum_{m_1 m_2}\langle l_2 m_2 LM\,|\,l_1 m_1\rangle\langle(\vec{r}_1\cdot\nabla_i)^2\psi^{(-)}(\alpha\,\vec{r}_i)\varphi_{j_2}^{l_2 m_2}(\vec{r}_2)\,|\,V(\vec{r}_1)\,|\,\varphi_{j_1}^{l_1 m_1}(\vec{r}_1)\psi^{(+)}(\vec{r}_i)\rangle\ , \tag{5}$$

the second order recoil DWBA amplitude. In a method analogous to but somewhat more involved than the evaluation of the first order recoil amplitude, standard angular momentum techniques will be exploited. If $\vec{r}_1$ is written in spherical coordinates

$$\vec{r}_1 = \sum_\mu (-1)^\mu\, r_1 (\tfrac{1}{3}4\pi)^{1/2}\, Y_1^\mu(\hat{r}_1)\,\hat{\xi}_{-\mu} \tag{6}$$

and the partial wave expansion is used for $\psi^{(-)*}$

$$\psi^{(-)*}(\alpha\,\vec{r}_i) = 4\pi\sum_{l'm'} i^{-l'}\,Y_{l'}^{m'}(\hat{k}_f)\,Y_{l'}^{m'*}(\hat{r}_i)\,f_{l'}(\alpha\,r_i)\ , \tag{7}$$

then we may apply the gradient formula[6]

$$\hat{\xi}_{-\mu}\cdot\nabla_i\, f_{l'}(\alpha\,r_i)\,Y_{l'}^{m'*}(\hat{r}_i) = -(1)^{m'}\alpha\Bigg[\left(\frac{l'+1}{2l'+3}\right)^{1/2}\langle l'-m'1-\mu\,|\,l'+1-m'-\mu\rangle\,Y_{l'+1}^{-m'-\mu}(\hat{r}_i)\left(\frac{df_{l'}(\alpha\,r_i)}{d(\alpha\,r_i)}-\frac{l'}{\alpha r_i}\,f_{l'}(\alpha r_i)\right)$$
$$-\left(\frac{l'}{2l'-1}\right)^{1/2}\langle l'-m'1-\mu\,|\,l'-1-m'-\mu\rangle\,Y_{l'-1}^{-m'-\mu}(\hat{r}_i)$$
$$\times\left(\frac{df_{l'}(\alpha r_i)}{d(\alpha r_i)}+\frac{l'+1}{\alpha r_i}\,f_{l'}(\alpha r_i)\right)\Bigg] \tag{8}$$

twice, in sequence, to Eq. (5). It turns out to be convenient to group the $\hat{r}_1$ angular dependence of the initial bound state wave function with the $\hat{r}_1$ angular dependence in the operator $(\vec{r}_1\cdot\nabla_i)^2$. After some tedious but straightforward algebra, one arrives at the following expression based on Eqs. (6), (7), and (8):

$$Y_{l_1}^{m_1}(r_1)\,(r_1\cdot\nabla_i)^2\psi^{(-)*}(\alpha r_i) = 4\pi\alpha^2\sum_{l'm'} i^{-l'}Y_{l'}^{m'}(\hat{k}_f)(-1)^{m'}r_1^{\,2}$$
$$\times\Bigg[\Bigg(\sum_{M'}(-1)^{M'}\Big[C^2_{l_1-2}\langle l_1 m_1 2M'\,|\,l_1-2m_1+M'\rangle\,Y_{l_1-2}^{m_1+M'}(\hat{r}_1)$$
$$+C^2_{l_1}\langle l_1 m_1 2M'\,|\,l_1 m_1+M'\rangle\,Y_{l_1}^{m_1+M'}(\hat{r}_1)$$
$$+C^2_{l_1+2}\langle l_1 m_1 2M'\,|\,l_1+2m_1+M'\rangle\,Y_{l_1+2}^{m_1+M'}(\hat{r}_1)\Big]$$
$$\times\Big[D^2_{l'-2}(\alpha r_i)\langle l'm'2-M'\,|\,l'-2-m'-M'\rangle\,Y_{l'-2}^{-m'-M'}(\hat{r}_i)$$
$$+D^2_{l'}(\alpha r_i)\langle l'-m'2-M'\,|\,l'-m'-M'\rangle\,Y_{l'}^{-m'-M'}(\hat{r}_i)$$
$$+D^2_{l'+2}(\alpha r_i)\langle l'-m'2-M'\,|\,l'+2-m'-M'\rangle\,Y_{l'+2}^{-m'-M'}(\hat{r}_i)\Big]\Bigg)$$
$$+C^0_{l_1}\langle l_1 m_1 00\,|\,l_1 m_1\rangle\,Y_{l_1}^{m_1}(\hat{r}_1)D^0_{l'}(\alpha r_i)\langle l'-m'00\,|\,l'-m'\rangle\,Y_{l'}^{-m'}(r_i)\Bigg]\ , \tag{9}$$

where

$$C^2_{l_1-2}=\left(\frac{l_1(l_1-1)}{(2l_1-1)(2l_1-3)}\right)^{1/2}, \tag{10}$$

$$C^2_{l_1}=-\left(\frac{2}{3}\right)^{1/2}\left(\frac{l_1^2+l_1}{4l_1^2+4l_1-3}\right)^{1/2}, \tag{11}$$

$$C^2_{l_1+2}=\left(\frac{(l_1+1)(l_1+2)}{(2l_1+3)(2l_1+5)}\right)^{1/2}, \tag{12}$$

$$C^0_{l_1}=-\frac{1}{(3)^{1/2}}, \tag{13}$$

and

$$D^2_{l'-2}(\alpha r_i)=\left(\frac{l'(l'-1)}{(2l'-1)(2l'-3)}\right)^{1/2}\left(\frac{d^2f_{l'}}{d(\alpha r_i)^2}+\frac{(2l'+1)}{\alpha r_i}\frac{df_{l'}}{d(\alpha r_i)}+\frac{(l'^2-1)}{(\alpha r_i)^2}f_{l'}\right), \tag{14}$$

$$D^2_{l'}(\alpha r_i)=-\left(\frac{2}{3}\right)^{1/2}\left(\frac{l'^2+l'}{4l'^2+4l'-3}\right)^{1/2}\left(\frac{d^2f_{l'}}{d(\alpha r_i)^2}+\frac{2}{\alpha r_i}\frac{df_{l'}}{d(\alpha r_i)}-\frac{l'(l'+1)}{(\alpha r_i)^2}f_{l'}\right), \tag{15}$$

$$D^2_{l'+2}(\alpha r_i)=\left(\frac{(l'+1)(l'+2)}{(2l'+3)(2l'+5)}\right)^{1/2}\left(\frac{d^2f_{l'}}{d(\alpha r_i)^2}-\frac{(2l'+1)}{\alpha r_i}\frac{df_{l'}}{d(\alpha r_i)}+\frac{l'(l'+2)}{(\alpha r_i)^2}f_{l'}\right), \tag{16}$$

$$D^0_{l'}(\alpha r_i)=-\frac{1}{(3)^{1/2}}\left(\frac{d^2f_{l'}}{d(\alpha r_i)^2}+\frac{2}{\alpha r_i}\frac{df_{l'}}{d(\alpha r_i)}-\frac{l'(l'+1)}{(\alpha r_i)^2}f_{l'}\right). \tag{17}$$

The operator $(\vec{r}_1\cdot\nabla_i)^2$ acts in a parallel manner on the bound state angular momentum eigenstate $Y^{m_1}_{l_1}(\hat{r}_1)$ and the partial wave scattering angular momentum states $Y^{m'}_{l'}(\hat{r}_i)$, effectively coupling each with quadrupole operators and a monopole operator.

Now Eq. (9) may be substituted into Eq. (5) to obtain

$$I^{l_1l_2LM}_{(2)}=2\pi\gamma^2\sum_{l'm'}(-1)^{m'}i^{-l'}\,Y^{m'}_{l'}(\hat{k}_f)\int\left(\frac{M_A+M_N}{M_A}\right)^3 d\vec{r}_i$$
$$\times\sum_{\substack{\Lambda M'\\ l''}}(-1)^{M'}D^{\Lambda}_{l'l''}(r_i)\langle l'-m'\Lambda-M'\,|\,l''-m'-M'\rangle\,Y^{m'+M'*}_{l''}(\hat{r}_i)F^{L\Lambda l_1''}_{MM'}(\vec{r}_i)\psi^{(+)}(\vec{r}_i), \tag{18}$$

where the second order modified "radial wave functions" $D^{\Lambda}_{l'l''}(r_i)$ are nonzero only for the l'', Λ values specified in Eqs. (14)–(17), and

$$F^{L\Lambda l_1''}_{MM'}(\vec{r}_i)=\sum_{\substack{m_1m_2\\ l_1''}}\langle l_2m_2LM\,|\,l_1m_1\rangle C^{\Lambda}_{l_1''}\langle l_1m_1\Lambda M'\,|\,l_1''m_1+M'\rangle\int Y^{m_2*}_{l_2}(\hat{r}_2)\,Y^{m_1+M'}_{l_1''}(\hat{r}_1)\varphi_2(r_2)V(r_1)\varphi_1(r_1)r_1^2\,d\vec{r}_2, \tag{19}$$

the modified form factor, is nonzero only for those values of l_1'', Λ specified in Eqs. (10)–(13). To evaluate $F^{L\Lambda l_1''}_{MM'}(\vec{r}_i)$, the identity

$$\vec{r}_1=\frac{M_A+M_N}{M_A}(\vec{r}_i-\vec{r}_2)$$

is applied, and then the integration over $\vec{r}_2$ may be carried out using the Sawaguri-Tobocman[7] expansion. The result takes the form

$$\int Y^{m_2*}_{l_2}(\hat{r}_2)\,Y^{m_1+M'}_{l_1''}(\hat{r}_1)\varphi_2(r_2)V(r_1)\varphi_1(r_1)r_1^2d\vec{r}_2=\sum_{\lambda}8\left(\frac{(2\lambda+1)(2l_1''+1)}{4\pi(2l_2+1)}\right)^{1/2}\langle\lambda m_2-m_1-M'l_1''m_1+M'\,|\,l_2m_2\rangle$$
$$\times\langle\lambda0l_1''0\,|\,l_20\rangle\,Y^{m_2-m_1-M'}_{\lambda}(\hat{r}_i)\bar{F}^{l_1''}_{\lambda 1}(r_i), \tag{20}$$

where the specific radial form of $\bar{F}^{l_1''}_{\lambda 1}(r_i)$ is calculated using modified harmonic oscillators.[7] After Eqs. (19) and (20) are substituted into Eq. (18), some Racah algebra must be performed to effect the sums over m_1, m_2, and M'. The partial wave expansion for $\psi^{(+)}(\vec{r}_i)$ is utilized for a quantization axis along the direction of the incoming beam

$$\psi^{(+)}(\vec{r}_i)=\sum_l i^l[4\pi(2l+1)]^{1/2}Y_l^0(\hat{r}_i)f_l(r_i)\ . \tag{21}$$

The final expression obtained for the second order recoil amplitude is

$$I_{(2)}^{l_1 l_2 LM}=\frac{\gamma^2}{2\alpha^2}\left(\frac{M_A+M_N}{M_A}\right)^3\sum_{ll'\lambda l''\Lambda} 8\left(\frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)}\right)^{1/2} i^{l-l'}(4\pi)^{3/2}$$
$$\times Y_{l'}^{M}(\hat{k}_f)(-1)^{l_1-\lambda-M}\left(\frac{(2\Lambda+1)(2l''+1)(2\lambda+1)}{4\pi(2L+1)}\right)^{1/2}$$
$$\times\langle l'ML-M\,|\,l0\rangle\langle l''0\lambda0\,|\,l0\rangle U(l'\Lambda l\lambda;l''L)\int dr_i r_i^2 B_\lambda^\Lambda(r_i)D_{l'l''}^\Lambda(r_i)f_l(r_i)\ , \tag{22}$$

where

$$B_\lambda^\Lambda(r_i)=\sum_{l_1''}\left(\frac{(2l_1''+1)}{(2\Lambda+1)}\right)^{1/2}C_{l_1''}^\Lambda\langle l_2 0 l_1''\,|\,\lambda0\rangle U(l_1 l_2\Lambda\lambda;Ll_1'')\bar{F}_\lambda^{l_1''}(r_i)\ . \tag{23}$$

This expression in many ways shows similarities to the first order recoil amplitude of Eq. (21) in Ref. 1. The fundamental difference is that in contrast to the dipole couplings of the first order expression, one now has monopole and quadrupole couplings in the Λ which may take values of 0, 2.

III. COMPUTATION

Although the derived expressions seem somewhat inelegant, they are quite suitable for rapid machine computation. Only one dimensional integrals are ever done numerically. After the rapid Sawaguri-Tobocman method is used for the bound state integration only four one dimensional form factors $[B_\lambda^\Lambda(r_i)]$ need be saved for the second order terms. Adding to this the two first order form factors and the no-recoil form factor, one has, to second order, all the information of the bound state kernel contained in seven one dimensional radial arrays.

The derived expression for the second order recoil amplitude has been incorporated into a heavy-ion DWBA code SRC (second order recoil code). SRC is based on the no-recoil code RDRC[5] and incorporates the first order recoil terms of Ref. 1 as well as the $(\alpha-\beta)$ terms implied by Eq. (4). First derivatives of radial wave functions [such as are required for evaluation of the functions $D_{ll'}^\Lambda(r_i)$] are calculated numerically for each partial wave. For evaluation of the second derivatives in the $D_{ll'}^\Lambda(r_i)$, the radial Schrödinger equation is utilized.

The code SRC has been tested for accuracy in a comparison with the exact finite range code LOLA[4] which utilizes the in principle exact method of Austern *et al.*[8] The comparisons indicated that, at energies of a few tens of MeV above the Coulomb barrier, single nucleon transfers calculated with SRC are essentially identical in angular shape and very close in absolute magnitude to those calculated with exact finite range. For example, in calculating the ^{88}Sr(^{16}O, ^{15}N)^{89}Y reaction for $L=0$ and $L=5$ at energies of 44, 46, 48, 50, 52, 56, and 59 MeV the greatest deviation between SRC and exact finite range calculations was 2.1%.[3] Even for the very poorly Q matched reactions ^{30}Si(^{16}O, ^{15}N)^{29}Al where no-recoil calculations failed by as much as a factor of 4, the SRC calculations were accurate to a few percent.[3]

The range of usefulness of the second order calculations is indicated by consideration of the expansion parameter $\gamma/\alpha\,\vec{r}_1\cdot\nabla_i\approx\gamma/\alpha\,\vec{r}_1\cdot\vec{k}$, where $\vec{k}$ is the scattering state local momentum. In a second order calculation the error is of the order $\frac{1}{6}(\gamma/\alpha\,\vec{r}_1\cdot\vec{k})$.[3] This term may be estimated by observing that

$$\frac{\gamma}{\alpha}\approx\frac{M_N}{\mu}\ ,$$

where M_N is the transferred mass and μ is the scattering system reduced mass

$$k=0.22[\,\mu(E-E_{\text{Coul}})]^{1/2}\ ,$$

where E is the outgoing particle c.m. energy, and

$$r_1\approx 3\text{ fm}.$$

Including an angle averaging factor one obtains

$$\frac{1}{3!}\left(\frac{\gamma}{\alpha}\,\vec{r}_1\cdot\vec{k}\right)^3\approx 0.01\left(\frac{E-E_{\text{Coul}}}{\mu}\right)^{3/2}M_N{}^3\ , \tag{24}$$

where E is in MeV and μ, M_N are in amu. These considerations must be viewed as only a rough estimate of the region of applicability of this method. However, it is clear that at one MeV per nucleon above the Coulomb barrier the method should be quite accurate for single nucleon

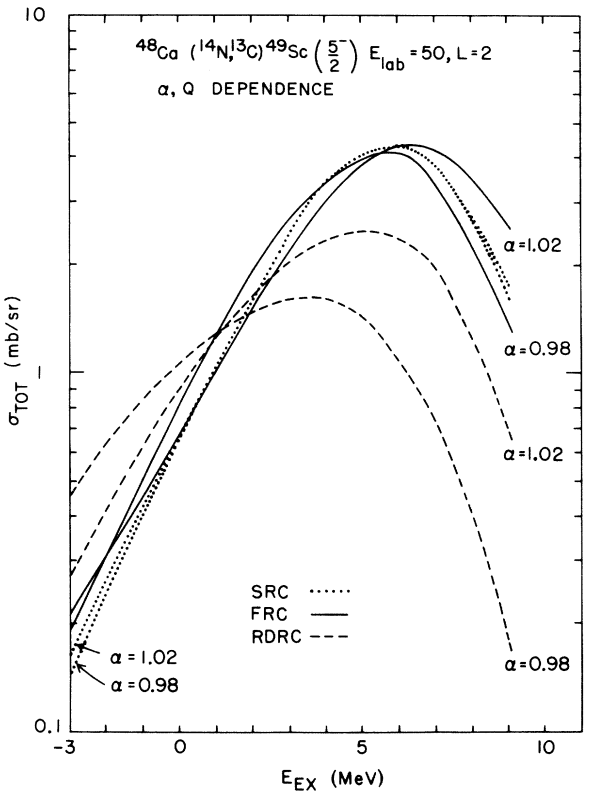

FIG. 2. Q dependence of ^{48}Ca(^{14}N, ^{13}C)^{49}Sc ($\frac{5}{2}^-$) at 50 MeV for two values of the expansion parameter α. RDRC is the no-recoil, FRC the first order recoil, and SRC the second order recoil calculation.

transfer [$\frac{1}{6}(\gamma/\alpha\,\vec{r}_1\cdot\vec{k})^3 \approx 0.01$], while the expansion will eventually break down at much higher energies and will have an error ~ 64 times larger for α particle transfer than for single nucleon transfer.

A final internal check on the convergence of the method may be made by varying the expansion parameter α in Eq. (4). It has been argued[1] that a physical range for α is $\beta < \alpha < \beta + \gamma R_1/(R_1+R_2)$ where R_1 and R_2 are projectile and target radii. Figure 2 shows computations done for a case particularly sensitive to recoil effects: ^{48}Ca (^{14}N, ^{13}C)^{49}Sc($\frac{5}{2}^-$) at 50 MeV (see Ref. 1). The curves show the α dependence of the no-recoil, first order, and second order total cross sections vs Q. The great variance with α in no recoil is reduced to a few percent in first order and almost eliminated in second order.

IV. DISCUSSION

The proper second order recoil calculation of heavy-ion DWBA single nucleon transfer cross sections has proved to be of significant utility. Since the savings of time over exact finite range calculations can be at least an order of magnitude, one is effectively allowed to do more calculations. This has proved useful both in data analysis[9] and in computer experiments, e.g., probing the nature of optical potentials.[10]

The region of applicability of the second order recoil method, although limited, covers a large class of cases of experimental interest. Since the convergence depends roughly only on the energy per nucleon, this method can be used even for reactions between quite massive nuclei such as those induced with Ar or Kr beams.[11] In any case the M_N factor in the expansion parameter seems to limit the region of applicability to single nucleon transfer reactions. In particular, comparisons with exact finite range calculations have shown the second order recoil method to be inadequate for α particle transfer.[3]

Finally it is worth observing that one need not stop at second order in the Taylor series. One could continue the series to higher orders to approach the accuracy of exact finite range. This has, in fact, been done by Braun-Munzinger and Harney[12] with, however, the additional approximations of replacing a bound state wave function with a spherical Hankel function and using a constant local momentum in place of the gradient operator. Carrying the Taylor series to higher order without any approximations would be more involved but straightforward. By use of the Schrödinger equation all the higher powers of the gradient operator could be expressed in terms of the radial wave functions, the first derivatives of the radial wave functions, and the appropriate higher derivatives of the radial potential. The advantage of such a method would be that an approach to exact finite range could be made which only involved one dimensional integrals and one dimensional form factors. The disadvantages would be the increasing complexity of the expressions for higher order terms along with the increasing numbers of form factors to be computed and saved by the computer for the radial integrations. Perhaps a point would come when the conventional exact finite range method would be more economical. However, with the continuing importance of numerical reaction calculations in nuclear physics, further investigation of a proper higher order Taylor series approach to recoil may prove to be fruitful.

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