ON THE CALCULATION OF NEUTRON TUNNELLING CROSS SECTIONS

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Abstract

We present an accurate expression for the matrix element for neutron tunnelling reactions using Hulthen wavefunctions for both initial and final neutron states and a Hulthen form for the neutron-binding potential (previous work is confined to asymptotic neutron wavefunctions and zero-range potentials).

This work is applied to the neutron tunnelling reaction $^{14}N(^{14}N, ^{13}N)^{15}N$. It is also employed to effect a retrospective justification for the rather empirical approximation used by May and Clayton (1968) in their explanation of the astrophysically interesting reaction $^{3}He(^{3}He, 2p)^{4}He$.

I. Introduction

The neutron tunnelling mechanism for nuclear reactions at low energies was first developed by Breit and co-workers (Breit and Ebel 1956*a*, 1956*b*; Breit 1964; Breit, Chun, and Wahsweiler 1964). The physical idea underlying this reaction mechanism is that a neutron "tunnels" from its initial state (in one nucleus) to its final state (in another nucleus), even though the incident and target nuclei are significantly far apart.

Calculations based on this idea were first applied, with striking success, to explain the interference pattern in the angular distribution in the reaction $^{14}N(^{14}N, ^{13}N)^{15}N$ (Hiebert, McIntyre, and Couch 1965, and references therein). More recently the mechanism has been invoked by May and Clayton (1968) to explain the behaviour of the reaction $^{3}He(^{3}He, 2p)^{4}He$ at very low energies. This latter reaction is of considerable current interest in astrophysics, as it plays an important role in determining the flux of neutrinos from the Sun (Bahcall 1969, and references therein).

In the present paper, we make some mathematical comments on the calculation of neutron tunnelling amplitudes. We go beyond previous work to use Hulthen wavefunctions (instead of the usual asymptotic wavefunctions) for both initial and final neutron states, and to use the corresponding Hulthen potential (instead of the usual zero-range potential) in calculating the relevant matrix element. This work is set out in Section II. Some applications of our more accurate matrix elements are outlined in Section III and the overall results are discussed briefly in Section IV.

II. Evaluation of the Matrix Element using Hulthen Wavefunctions

We consider the neutron tunnelling process whereby a target nucleus of charge Z_2 and mass number B is bombarded by particles of charge Z_1 and mass number $A+1$, with the target capturing a neutron to give a final nucleus of mass $B+1$ and an outgoing particle of mass number A.

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If the incident energy is well below the Coulomb barrier for the process, we may use pure Coulomb wavefunctions $F_{\rm i}^{(+)}$ and $F_{\rm f}^{(-)}$ for the initial and final *scattering* states (i.e. nuclear forces may be neglected). Furthermore, we take the incident and target nuclei to be massive ($A \to \infty$, $B \to \infty$). The neutron tunnelling matrix element can now be written in what is, in effect, distorted-wave Born approximation:

$$T(\theta) = \langle F_{\rm f}^{(-)}(\boldsymbol{r})\,\chi_{\rm f}(\boldsymbol{r}')\,|\,V_{\rm ni}\,|\,\chi_{\rm i}(\boldsymbol{r}-\boldsymbol{r}')\,F_{\rm i}^{(+)}(\boldsymbol{r})\rangle\,, \tag{1}$$

where $\chi_{\rm i}$ and $\chi_{\rm f}$ are the initial and final bound-neutron wavefunctions, $\boldsymbol{r}$ is the distance between the nuclei A and B, and $\boldsymbol{r}'$ is the distance of the neutron from B. The term $V_{\rm ni}(\boldsymbol{r}-\boldsymbol{r}')$ is the potential binding the neutron in the initial nucleus, that is, the matrix element has been expressed in the so-called "prior" form. (The alternative use of the final state potential $V_{\rm nf}(\boldsymbol{r}')$ leads to the "post" form of the matrix element.)

Following the initial work of Breit and others, Buttle and Goldfarb (1966) have presented neutron tunnelling expressions which contain essentially the same physical assumptions, but with fewer mathematical approximations. The potential is taken to be of zero range, and asymptotic wavefunctions are used for the neutron states, chosen to be S states:

$$\chi(\boldsymbol{r}) = (N/r)\exp(-\gamma r)\,. \tag{2}$$

Here N is the normalization constant (which includes the spectroscopic factor) and $\gamma_{\rm i}$ and $\gamma_{\rm f}$ are the usual initial and final neutron binding energy wavenumbers. This leads to the approximation $T(\theta) \simeq N_{\rm i}\,N_{\rm f}\,I(\gamma_{\rm f}\,|\,\theta)$, where

$$I(\gamma\,|\,\theta) = \int F_{\rm f}^{(-)*}(\boldsymbol{r})\,r^{-1}\exp(-\gamma r)\,F_{\rm i}^{(+)}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \tag{3}$$

$$= 4\pi\exp\{-\tfrac{1}{2}(\eta+\eta')\}\frac{\{(\gamma-\mathrm{i}k)^2+k'^2\}^{\mathrm{i}\eta}\{(\gamma-\mathrm{i}k')^2+k^2\}^{\mathrm{i}\eta'}}{\{(k-k')^2+\gamma^2\}^{\mathrm{i}\eta'}\{\Delta^2+\gamma^2\}^{1+\mathrm{i}\eta}}$$

$$\times F\left(1+\mathrm{i}\eta,\,-\mathrm{i}\eta';\,1;\,\frac{2kk'(1-\cos\theta)}{\Delta^2+\gamma^2}\right). \tag{4}$$

We have chosen to write the matrix element (4) in the "prior" form. In fact, as has been shown by Buttle and Goldfarb (1966) and May and Clayton (1968), the angle dependence of the matrix element in prior form is identical with that in post form, and in the limit of infinitely massive nuclei we have the full identity (angle dependence and absolute magnitude) $I_{\rm post}(\theta) = I_{\rm prior}(\theta)$. The proof of these identities rests on the mathematical relationship

$$F(a,b;c;z) = (1-z)^{c-a-b}F(c-a,c-b;c;z)\,,$$

along with energy conservation.

In the expression (4) k and k' are respectively the initial and final centre-of-mass wavenumbers (that is, $E = \hbar^2k^2(A+B)/2mAB$) and η and η' are the initial and final state Coulomb parameters,

$$\eta = Z_1\,Z_2\,e^2mAB/(A+B)\hbar^2k\,. \tag{5}$$

When we say "below the Coulomb barrier" we mean $\eta > 1$. $F(a,b;c;z)$ is the usual hypergeometric function and $\Delta = |\boldsymbol{k}-\boldsymbol{k}'|$ is the momentum transfer.

As pointed out by May and Clayton (1968), it is a very straightforward matter to go beyond the asymptotic wavefunction for χ_{f} in equation (1), using instead the more accurate Hulthen wavefunction*

$$\chi = (N/r)\{\exp(-\gamma r)-\exp(-\beta r)\}. \tag{6}$$

The parameter β can be related to the range of the potential (Sachs 1953), or alternatively to the r.m.s. radius of the charge distribution. If we use (6) for χ_{f} but keep the zero-range form for $V_{\mathrm{ni}}\chi_{\mathrm{i}}$, the corresponding approximation to the matrix element ($\hat{I}(\gamma_{\mathrm{f}})$ say) obviously takes the form of a simple difference between two expressions such as (4):

$$\hat{I}(\gamma_{\mathrm{f}}\,|\,\theta) = I(\gamma_{\mathrm{f}}\,|\,\theta)-I(\beta_{\mathrm{f}}\,|\,\theta). \tag{7}$$

Now we proceed to present a new and more accurate expression for the amplitude $T(\theta)$, based on the use of Hulthen wavefunctions for *both* initial and final neutron states along with use of the corresponding Hulthen potential for V_{ni}.

First it is helpful to write down the Fourier transform of the Hulthen wavefunction (6),

$$\chi(\boldsymbol{\kappa}) = \frac{N}{2\pi^2}\left(\frac{1}{\gamma^2+\kappa^2}-\frac{1}{\beta^2+\kappa^2}\right), \tag{8a}$$

and the Fourier transform of the product $V\chi$,

$$\overline{V\chi}(\boldsymbol{\kappa}) = \frac{N}{2\pi^2}\left(1-\frac{\gamma^2+\kappa^2}{\beta^2+\kappa^2}\right). \tag{8b}$$

The matrix element (1) can now be written as

$$T(\theta) = \int F_{\mathrm{f}}^{(-)*}(\boldsymbol{r})\,F_{\mathrm{i}}^{(+)}(\boldsymbol{r})\,G(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}, \tag{9}$$

where G is the convolution integral of the Fourier transforms of χ_{f} and $\overline{V_{\mathrm{i}}\chi_{\mathrm{i}}}$:

$$G(\boldsymbol{r}) = (2\pi)^3\int \exp(-\mathrm{i}\,\boldsymbol{\kappa}\,.\,\boldsymbol{r})\,\chi_{\mathrm{f}}(\boldsymbol{\kappa})\,\overline{V\chi_{\mathrm{i}}}(\boldsymbol{\kappa})\,\mathrm{d}\boldsymbol{\kappa} \tag{10}$$

$$= N_{\mathrm{i}}N_{\mathrm{f}}\left(\frac{\beta_{\mathrm{i}}^2-\gamma_{\mathrm{i}}^2}{\beta_{\mathrm{i}}^2-\gamma_{\mathrm{f}}^2}\right)\left(\frac{\exp(-\gamma_{\mathrm{f}}r)}{r}-\frac{(\beta_{\mathrm{i}}^2-\gamma_{\mathrm{f}}^2)}{(\beta_{\mathrm{i}}^2-\beta_{\mathrm{f}}^2)}\frac{\exp(-\beta_{\mathrm{f}}r)}{r}-\frac{(\beta_{\mathrm{f}}^2-\gamma_{\mathrm{f}}^2)}{(\beta_{\mathrm{f}}^2-\beta_{\mathrm{i}}^2)}\frac{\exp(-\beta_{\mathrm{i}}r)}{r}\right). \tag{11}$$

We can now write down our final formula for the neutron tunnelling matrix element using a Hulthen potential and Hulthen wavefunctions for the neutron states:

$$T(\theta) = N_{\mathrm{i}}N_{\mathrm{f}}\frac{(\beta_{\mathrm{i}}^2-\gamma_{\mathrm{i}}^2)}{(\beta_{\mathrm{i}}^2-\gamma_{\mathrm{f}}^2)}\left(I(\gamma_{\mathrm{f}}\,|\,\theta)-\frac{(\beta_{\mathrm{i}}^2-\gamma_{\mathrm{f}}^2)}{(\beta_{\mathrm{i}}^2-\beta_{\mathrm{f}}^2)}I(\beta_{\mathrm{f}}\,|\,\theta)-\frac{(\beta_{\mathrm{f}}^2-\gamma_{\mathrm{f}}^2)}{(\beta_{\mathrm{f}}^2-\beta_{\mathrm{i}}^2)}I(\beta_{\mathrm{i}}\,|\,\theta)\right), \tag{12}$$

The quantities $I(\gamma\,|\,\theta)$ follow from the recipe given in equation (4).

* For a discussion of the use of Hulthen wavefunctions see Sachs (1953) or Ma (1954).

By a straightforward extension of the argument referred to after (4) above, we can again establish the identity of post and prior forms in the present infinitely massive limit: $T_{\text{post}}(\theta) = T_{\text{prior}}(\theta)$. This is reassuring, as such identities are often violated in approximate treatments of "exchange" reactions.

We now go on to apply formula (12) to some particular neutron tunnelling reactions.

III. Applications of the Theory

(a) *The Reaction* $^{14}N(^{14}N, ^{13}N)^{15}N$

We first apply expression (12) to the reaction $^{14}N(^{14}N, ^{13}N)^{15}N$, which has been extensively studied (using asymptotic neutron wavefunctions) by Breit and co-workers (Breit and Ebel 1956*a*, 1956*b*; Breit 1964; Breit, Chun, and Wahsweiler 1964) and by Buttle and Goldfarb (1966). The reaction has an essentially vanishing Q value; that is, $k = k'$, $\eta = \eta'$.

For neutron tunnelling reactions with small Q values, one can simplify the expression (4) for $I(\theta)$ by use of the identity

$$F(1+\mathrm{i}\eta, -\mathrm{i}\eta; 1; \Delta^2/(\Delta^2+\gamma^2)) \equiv P_{\mathrm{i}\eta}((\gamma^2-\Delta^2)/(\gamma^2+\Delta^2)),$$

followed by use of the asymptotic expression for Legendre polynomials of large order. In this way, May (1968) has shown that (4) leads to the somewhat more crudely approximate expression for the tunnelling amplitude obtained by Breit, Chun, and Wahsweiler (1964), plus corrections (amounting to about 3% for the experiments of Hiebert, McIntyre, and Couch 1965) arising from the more accurate treatment of the Coulomb scattering wavefunctions.

If we now turn to our more accurate expression (12), we similarly obtain further corrections to the work of Breit, Chun, and Wahsweiler (1964), arising now from corrections to the asymptotic neutron wavefunctions. Again using the simplifying procedure* of May (1968) to facilitate computation, these new corrections are found to have a relative magnitude of $0\cdot3$% for the experiments of Hiebert, McIntyre, and Couch (1965). (The parameter values appropriate to these experiments are $k = k' = 1\cdot538\ \mathrm{f}^{-1}$, $\eta = \eta' = 7\cdot748$, $\gamma_{\mathrm{i}} = 0\cdot713\ \mathrm{f}^{-1}$, and $\gamma_{\mathrm{f}} = 0\cdot724\ \mathrm{f}^{-1}$; the Hulthen parameters were taken as $\beta_{\mathrm{i}} = 2\cdot093\ \mathrm{f}^{-1}$ and $\beta_{\mathrm{f}} = 1\cdot890\ \mathrm{f}^{-1}$.)

Thus our refinements to the neutron wavefunctions are quite irrelevant in these experimental circumstances. The reason is that the Coulomb parameter is large enough to keep the incident and target nuclei (A and B) separated by a distance which is indeed substantially larger than the range of the neutron-binding potentials; thus an asymptotic description of the neutron wavefunction is quite accurate.

We now consider an example where the above conditions do not apply.

(b) *An Approximation to the Reaction* $^{3}He(^{3}He, 2p)^{4}He$

An explanation of the experimental results (Neng-Ming *et al.* 1966; Winkler and Dwarakanath 1967*a*, 1967*b*; Bacher and Tombrello 1968) for the $^{3}He(^{3}He, 2p)^{4}He$

* We do not give the explicit formula for $I(\beta\,|\,\theta)$ in the case $k = k'$, $\eta = \eta' > 1$, as these expressions (although much easier to compute than the hypergeometric functions) are very complicated, and are exactly analogous to those given in May (1968).

reaction at the low energies of interest to astrophysicists has been given by May and Clayton (1968), who invoke the neutron tunnelling mechanism. However, at the energies of interest here (around 0·1–1 MeV), the Coulomb parameters are not so large, due to the lightness (and consequent small charge) of the nuclei involved; in fact we are dealing with $\eta \sim \eta' \sim 2$. Consequently the non-asymptotic parts of the neutron wavefunction make significant contributions to the matrix element, and one wishes to use an accurate expression such as (12).

Unfortunately, the technique by which we arrived at (12) necessitates the assumption of infinitely massive nuclei, a limit which does not pertain to the light nuclei involved here.

TABLE 1

DEFINITIONS OF CROSS SECTIONS $\sigma_i = |T(\theta)+T(\pi-\theta)|^2$, $i = 1, 2, 3, 4$

σ_i	Initial State Neutron Wavefunction	Final State Neutron Wavefunction
$\sigma_1(\theta)$	Zero-range approximation (asymptotic wavefunction)	Zero-range approximation (asymptotic wavefunction)
$\sigma_2(\theta)$	Zero-range approximation	Hulthen wavefunction (prior form of $T(\theta)$)
$\sigma_3(\theta)$	Hulthen wavefunction (post form of $T(\theta)$)	Zero-range approximation
$\sigma_4(\theta)$	Hulthen wavefunction	Hulthen wavefunction

What is done in May and Clayton (1968) is as follows. First $\sigma_1(\theta)$ is defined to be the cross section calculated using asymptotic neutron wavefunctions throughout (i.e. equation (4)), $\sigma_2(\theta)$ to be the cross section with a Hulthen wavefunction for the final neutron state *only* (using the prior representation, i.e. equation (7)), and $\sigma_3(\theta)$ to be the cross section with a Hulthen wavefunction for the initial neutron state *only* (using the post representation). All these cross sections can be calculated along the lines laid down early in Section II, even for nuclei of finite mass. Next $\sigma_4(\theta)$ is defined to be the cross section calculated with Hulthen wavefunctions and Hulthen potentials throughout; with finite mass nuclei, evaluation of σ_4 is *not* possible (short of numerical integration of a complicated three-dimensional integral). These definitions of $\sigma_i(\theta)$ ($i = 1, 2, 3, 4$) are summarized in Table 1.

May and Clayton (1968) estimate the desired cross section σ_4 by the relation

$$\tilde{\sigma}_4 = \sigma_1(\sigma_2/\sigma_1)(\sigma_3/\sigma_1)\,. \tag{13}$$

That is, starting from the asymptotic wavefunction cross section σ_1, the fully accurate σ_4 is estimated as the *product* of the corrections introduced by first replacing one and then (separately) the other neutron wavefunction by a Hulthen form. This estimate provides the basis of May and Clayton's work.

Now, although the formula (12), pertaining to $\sigma_4(\theta)$ in the limit of infinitely massive nuclei, is not directly applicable to this particular neutron tunnelling reaction involving light nuclei, it certainly *is* able to provide us with a test of the reliability of the estimate (13) above. Accordingly, we take a set of sample parameters,

$$\left.\begin{array}{c} k = k' = 2\cdot164\ \mathrm{f}^{-1}, \qquad \eta = \eta' = 2\cdot00, \\ \gamma_{\mathrm{i}} = \gamma_{\mathrm{f}} = 1\cdot00\ \mathrm{f}^{-1}, \qquad \beta_{\mathrm{i}} = 2\cdot85\ \mathrm{f}^{-1}, \qquad \beta_{\mathrm{f}} = 3\cdot25\ \mathrm{f}^{-1}, \end{array}\right\} \tag{14}$$

and use the results of Section II to calculate σ_1 (from equation (4)), σ_2 (from (7)), σ_3 (from the post analogue of (7)), and σ_4 (from (12)). These results are shown in Table 2, and are compared with the estimate $\tilde{\sigma}_4$ provided by equation (13).

TABLE 2

CROSS SECTIONS $\sigma_i(\theta)$, $i = 1, 2, 3, 4$, AND ESTIMATE $\tilde{\sigma}_4(\theta)$

Note that the cross section is symmetric about $\theta = 90°$. The cross section σ_1 is in arbitrary units, as only the comparisons (σ_4/σ_1 etc.) are of interest here

θ	σ_1	σ_2/σ_1	σ_3/σ_1	σ_4/σ_1	$\tilde{\sigma}_4/\sigma_1$
0°	143	2·6	3·0	7·7	7·9
5	153	2·6	3·0	7·7	7·9
10	171	2·6	3·0	7·8	7·9
15	170	2·6	3·0	7·8	7·9
20	124	2·6	3·0	7·7	7·8
25	52	2·5	2·9	7·2	7·4
30	5	2·2	2·3	4·5	5·1
35	5	2·3	4·2	14·1	13·8
40	31	3·0	3·6	10·8	10·6
45	51	2·9	3·5	10·4	10·2
50	49	2·9	3·5	10·6	10·3
55	32	3·0	3·7	11·3	10·9
60	13	3·2	4·0	13·3	12·6
65	15	4·2	6·0	26·9	25·1
70	12	1·4	1·0	0·1	1·4
75	10	2·2	2·2	3·8	4·9
80	22	2·3	2·5	5·1	5·9
85	32	2·4	2·6	5·5	6·3
90	35	2·4	2·6	5·7	6·4

We see from the last two columns of Table 2 that the estimate $\tilde{\sigma}_4(\theta)$ to the accurate cross section $\sigma_4(\theta)$ is reliable to within 10% for all angles. This is true despite the fact that $\sigma_4(\theta)$ differs from $\sigma_1(\theta)$ by factors of as much as 20 or more.

We may also consider the results for the total cross sections

$$\tilde{\sigma}^{\mathrm{tot}} = \int_0^{\pi} \sigma(\theta) \sin\theta \, \mathrm{d}\theta\,. \tag{15}$$

For our example, we get

$$\sigma_1^{\mathrm{tot}} = 65\,, \qquad \sigma_4^{\mathrm{tot}} = 543\,, \qquad \tilde{\sigma}_4^{\mathrm{tot}} = 551\,,$$

where all the results are expressed in the same arbitrary units. We see that $\tilde{\sigma}_4$ is a very accurate estimate of σ_4, even though both differ markedly from the simple σ_1. These results may be taken as a retrospective justification of the work presented in May and Clayton (1968).

IV. Discussion

We have given an expression (equation (12)) for the neutron tunnelling amplitude based on accurate (non-asymptotic) neutron wavefunctions and potentials. As seen in the example in Section III(a), when the Coulomb parameters are large these corrections to the use of asymptotic neutron wavefunctions are not significant. However, as shown in the example in Section III(b), when the Coulomb parameters are of the order of unity the non-asymptotic parts of the neutron wavefunctions can make substantial contributions to the reaction matrix element. We have used the present accurate results to provide a justification for the rather empirical approximation (13) used by May and Clayton (1968) in their explanation of the astrophysically interesting reaction $^{3}He(^{3}He, 2p)^{4}He$.

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