Corrections to the Fermi approximation in neutron-nuclear scattering

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(Received 10 June 1983)

The Fermi approximation is fundamental in the use of thermal-neutron scattering to study solid-state and molecular physics. It is important to understand how accurate this approximation is. There have been a number of computations of corrections to the Fermi approximation for model systems. For some of these, however, the correction has been found to be divergent. This raises some questions about the validity of these calculations. Here we calculate the first-order correction to the Fermi approximation through an approach in which the scattering nucleus is replaced by a boundary condition. It is shown that the first-order correction to the Fermi approximation can always be made to converge and that the magnitude of the correction is small.

I. INTRODUCTION

The problem of neutron scattering from chemically bound nuclei is usually treated by the Fermi approximation, i.e., the first Born approximation plus the Fermi pseudopotential,[1]

$$V(\vec{r})=\frac{2\pi\hbar^2}{m}a\delta(\vec{r}) , \tag{1}$$

where m is the mass of the neutron, a is the bound-atom scattering length, and the scatterer is assumed to be located at the origin. The Fermi approximation is designed to give the correct, experimentally determined scattering length for neutron scattering from a free nucleus in the limit of zero neutron energy.

The first-order correction to the Fermi approximation has been the subject of several studies during the past four decades;[2–12] these studies have given some divergent results for this term. This is a direct result of the zero-range potential (1), which is used to describe the interaction, and creates doubts about the validity of the estimates of the magnitude of this term which have been calculated to be small. Of course, had the real potential been used, the results for the correction terms would be finite. However, such computations are not possible. The question remains however, whether one can develop a reasonable, finite series of approximations for a zero-range potential, i.e., treating the nucleus as a boundary condition on the neutron wave function.

In this study we use a modified version of the zero-range interaction potential to develop a consistent method which leads to the convergence of the first-order correction term for all systems. This approach is then applied to some specific systems which have been studied earlier. Here we treat neither resonant scattering nor multiple scattering. These have been dealt with extensively by other authors.[13]

II. NEUTRON-NUCLEAR INTERACTION

Consider neutron scattering from a single, bound nucleus. It is clear that the Schrödinger equation has no solution for a potential of the form of Eq. (1). A number of authors have suggested the use of a different pseudopotential to replace the Fermi pseudopotential;[9–11]

$$V(\vec{r})=\frac{2\pi\hbar^2}{m}a\delta(\vec{r})\frac{\partial}{\partial r}r . \tag{2}$$

For this potential the Schrödinger equation does have a solution. It is noted that Eq. (2), acting on a nonsingular wave function, gives the same result as the Fermi pseudopotential, but acting on a singular wave function of the $1/r$ type, it removes the singularity.

III. SCATTERING (T) MATRIX EXPANSION

The T matrix is determined by the solution of

$$T=V+VGT , \tag{3}$$

where

$$G=(E-H_0+i\epsilon)^{-1} , \tag{4}$$

where E is the total energy of the system and H_0 is its Hamiltonian in the absence of neutron-nuclear interactions. A series expansion for T can be written as

$$T=(1-VG_0)^{-1}\sum_{s=0}^{\infty}[(VG-VG_0)(1-VG_0)^{-1}]^sV , \tag{5}$$

where

$$G_0=\left[\frac{-p_n^2}{2\mu_0}+i\epsilon\right]^{-1} \tag{6}$$

or

$$T=T_0+T_1+T_2+\cdots , \tag{7}$$

where

$$T_0=(1-VG_0)^{-1}V \tag{8}$$

and

$$T_1=(1-VG_0)^{-1}(VG-VG_0)(1-VG_0)^{-1}V \tag{9}$$

etc.

The first term in this expansion gives the Fermi pseudopotential approximation. Consider a neutron, scattering from a single, free nucleus. Using the pseudopotential for the interaction between the neutron and the nucleus, the Hamiltonian for this system in the center-of-mass frame is

$$H=-\frac{p_n^2}{2\mu}+V(\vec{r}_n-\vec{r}_N)\ , \tag{10}$$

where μ is the reduced mass of the neutron and the nucleus with masses m and m_1, respectively, and $\vec{r}_n$ and $\vec{r}_N$ are the vector positions of the neutron and the nucleus, respectively. We have for this system

$$T=V+VG_1T \tag{11}$$

where

$$G_1=\left[E-\frac{p_n^2}{2\mu}+i\epsilon\right]^{-1}\ , \tag{12}$$

and where E is the total energy of the system. We are interested in determining off the energy shell results for $Te^{i\vec{k}\cdot\vec{r}}n$. That is, we need this for cases in which E does not equal $\hbar^2k^2/2\mu$. It can be shown that the matrix elements of T are exactly given by

$$\langle e^{i\vec{k}'\cdot\vec{r}_n}\mid T\mid e^{i\vec{k}\cdot\vec{r}_n}\rangle=\frac{2\pi\hbar^2}{m}a\frac{e^{i(\vec{k}-\vec{k}')\cdot\vec{r}_N}}{1+iKa}\ , \tag{13}$$

where $K=(2\mu E/\hbar^2)$ for a potential of the form of Eq. (2), even off the energy shell. Comparing Eqs. (8) and (6) with Eqs. (11) and (12), it becomes clear that the matrix elements of the transition operator T_0 are given by the $E\rightarrow 0$ limit of (13), or

$$\langle e^{i\vec{k}'\cdot\vec{r}_n}\mid T_0\mid e^{i\vec{k}\cdot\vec{r}_n}\rangle=\frac{2\pi\hbar^2}{m}ae^{i(\vec{k}-\vec{k}')\cdot\vec{r}_N}\ . \tag{14}$$

Taking matrix elements of Eq. (14) between atomic states will result in the Fermi approximation,

$$T_{ofi}=\frac{2\pi\hbar^2}{m}a\langle\phi_f\mid e^{i(\vec{k}-\vec{k}')\cdot\vec{r}_N}\mid\Phi_i\rangle\ . \tag{15}$$

Therefore, the matrix elements of the first term in the scattering matrix expansion (5) give the Fermi approximation, and this is obtained by taking the exact limit at $E\rightarrow 0$ off the energy-shell T-matrix elements corresponding to a free nucleus between the initial and final states of the system. It is of interest that this first term (the Fermi approximation) is independent of μ. Therefore, μ does not have to be the reduced mass of the neutron and the scatterer as proposed by others and it may be chosen at our convenience. We will choose this parameter so that the convergence of the first-order correction term is assured and call it μ_0.

IV. FIRST-ORDER CORRECTION TO THE FERMI APPROXIMATION

Let us now compute the first-order correction to the Fermi approximation for several model systems. We begin by considering the problem of a neutron, scattering from a single bound atom (or more exactly from a single bound nucleus). The Hamiltonian of the atom, including the binding potential, will be denoted by H_A. We label the eigenfunctions of $p_n^2/2m$ and H_A as

$$\begin{aligned}&(p_n^2/2m)e^{i\vec{k}_l\cdot\vec{r}_n}=E_le^{i\vec{k}_l\cdot\vec{r}_n}\ ,\\ &H_A\phi_j(\vec{r}_N)=E_j\phi_j(\vec{r}_N)\ ,\end{aligned} \tag{16}$$

where the indices l and j identify the intermediate states of the neutron and the nucleus, respectively. We also define the total Hamiltonian of the system in the absence of neutron-nucleus interaction

$$H_0=p_n^2/2m+H_A\ . \tag{17}$$

The first-order correction transition operator is given by Eq. (9). The matrix elements of T_1 are determined by including the set of intermediate eigenstates of H_0,

$$T_{1fi}=\left[\frac{2\pi\hbar^2a}{m}\right]^2(X)\sum_l\langle\phi_f\mid e^{i(\vec{k}_l-\vec{k}')\cdot\vec{r}_N}\mid\phi_j\rangle\langle\phi_j\mid e^{-i(\vec{k}_l-\vec{k})\cdot\vec{r}_N}\mid\phi_j\rangle(G_{jl}-G_{0l})\ , \tag{18}$$

where

$$G_{jl}=\left[E-E_j-\frac{\hbar^2k_l^2}{2m}+i\epsilon\right]^{-1}$$

and

$$G_{0l}=\left[-\frac{\hbar^2k_l^2}{2\mu_0}+i\epsilon\right]^{-1}\ . \tag{19}$$

The question of existence and convergence of the first-order correction term has been the subject of a number of studies.[2–8] Now, we will consider this problem. Our analysis will be based on the following central argument. Since the first term of the T-matrix expansion series is independent of μ_0, we may therefore choose this parameter at our convenience. We will choose it so that the convergence of the first-order correction is ensured.

A. A particle harmonically bound in a finite mass

In this section we consider scattering from a nucleus bound, harmonically, in a molecule of finite mass. We assume that the neutron interacts only with the scattering particle and not with the rest of the molecule which we will call the binding particle.

Let us define some center-of-mass variables before we

proceed to do the calculations for this system. m_1 is the mass of the scatterer. m_2 is the mass of the binding particle. $M=m_1+m_2$ is the total mass of the molecule. $\vec{r}_1$ is the vector position of the scattering particle. $\vec{r}_2$ is the vector position of the binding particle. $\mu_1=m_1m_2/(m_1+m_2)$ is the reduced mass of the scatterer and the binding particle. $\vec{r}=\vec{r}_1-\vec{r}_2$ is the relative coordinate. $\vec{R}=(m_1\vec{r}_1+m_2\vec{r}_2)/M$ is the center-of-mass coordinate. $V_s(\vec{r})$ is the interaction potential binding the scatterer. $\phi_i(\vec{r}),\phi_f(\vec{r})$ are the initial and final states of the scatterer in relative coordinates. $\vec{k},\vec{k}'$ are the initial and final wave vectors of the neutron. l,j,s are the indices corresponding to intermediate states of the neutron, the scatterer, and the center of mass. $\vec{p}_1,\vec{p}_2$ are the momenta of the scatterer and the binding particle. $\vec{p}=\vec{p}_1+\vec{p}_2$ is the momentum of the center of mass. $\vec{p}=(m_2\vec{p}_1-m_1\vec{p}_2)/M$ is the relative momentum.

The Schrödinger equation for this system may now be written as

$$\left[\frac{P^2}{2M}+\frac{P^2}{2\mu_1}+V_s(\vec{r})\right]\Psi(\vec{r},\vec{R})=E\Psi(\vec{r},\vec{R})\ . \tag{20}$$

We look for solutions such that

$$\Psi(\vec{r},\vec{R})=\phi(\vec{r})\Phi(\vec{R})\ . \tag{21}$$

Using (21) in (20) we find two equations describing the system in the center of mass and relative coordinates

$$-\frac{\hbar^2}{2M}\Delta_R\Phi(\vec{R})=E_R\Phi(\vec{R}) \tag{22}$$

and

$$\left[-\frac{\hbar^2}{2\mu_1}\Delta_r+V_s(\vec{r})\right]\Phi(\vec{r})=E_r\phi(\vec{r})\ , \tag{23}$$

where the total energy of the system is given by

$$E=E_R+E_r\ . \tag{24}$$

Equation (22) has a plane-wave solution of the form

$$\Phi(\vec{R})=e^{i\vec{K}\cdot\vec{R}} \tag{25}$$

with

$$K=\left[\frac{2ME_R}{\hbar^2}\right]^{1/2}\ . \tag{26}$$

The first correction to the Fermi approximation for this system is given by

$$T_{1fi}=\sum_{jls}\left[\frac{2\pi\hbar^2}{m}\right]^2\langle\Psi_f\,|\,e^{i(\vec{k}_l-\vec{k}')\cdot\vec{r}_1}\,|\,\Psi_j\rangle \times\langle\Psi_j\,|\,e^{i(\vec{k}-\vec{k}_l)\cdot\vec{r}_1}\,|\,\Psi_i\rangle(G_{jls}-G_{0l0})\ , \tag{27}$$

where

$$G_{jls}=\left[E-\frac{\hbar^2K_j^2}{2M}-E_j-\frac{\hbar^2k_l^2}{2m}+i\epsilon\right]^{-1}\ , \tag{28}$$

$$G_{0l0}=\left[-\frac{\hbar^2k_1^2}{2\mu_0}+i\epsilon\right]^{-1}\ , \tag{29}$$

and

$$\phi(\vec{r})=\prod_i\phi_i(r_i)\ ,$$

where $r_1=x$, $r_2=y$ and $r_3=z$ in cartesian coordinates, and ϕ_i is the wave function of a linear harmonic oscillator

$$\phi_{n_i}(r_i)=\pi^{-1/4}(b_i)^{1/2}\frac{e^{-r_i^2/2b_i^2}}{(2^{n_i}n_i!)^{1/2}}H_{n_i}(r_i/b_i)\ ,$$

where

$$b_i=\left[\frac{\hbar}{\mu_1\omega_i}\right]^{1/2}\ . \tag{30}$$

Carrying out the sum over s and l we find[12]

$$T_{1fi}=-\frac{2\pi\hbar^2a^2}{m}\sum_j\int\int d^3r\,d^3r'e^{-i\alpha\vec{k}'\cdot\vec{r}}\phi_f^*(\vec{r})\phi_j(\vec{r})e^{i\alpha\vec{k}\cdot\vec{r}'} \times\phi_j^*(\vec{r}')\phi_i(\vec{r}')\left[e^{i\alpha\vec{C}\cdot(\vec{r}-\vec{r}')}\frac{(2\mu'/m)e^{i\alpha q_j'|\vec{r}-\vec{r}'|}}{\alpha|\vec{r}-\vec{r}'|}-\frac{2\mu_0/m}{\alpha|\vec{r}-\vec{r}'|}\right]\ , \tag{31}$$

where

$$\mu'=\frac{mM}{m+M}\ ,$$
$$\vec{C}=\frac{\mu'}{M}(\vec{K}+\vec{k})\ , \tag{32}$$
$$q_j'=\left[\frac{2\mu'}{\hbar^2}(E-E_j)-\frac{\mu'}{m+M}(\vec{K}+\vec{k})^2\right]^{1/2}\ ,$$

and

$$\alpha=m_2/M\ .$$

For thermal-neutron scattering ($k \simeq 0$) from a proton ($m = m_1$), harmonically bound in a molecule of total mass M, (31) reduces to

$$T_{1fi} = -\frac{\pi\hbar^2 a^2}{m} \sum_j \int\int d^3r\, d^3r'\, \phi_f^*(\vec{r})\phi_j(\vec{r})\phi_j^*(\vec{r}')\phi_i(\vec{r}') \left[\frac{(2\mu'/m)e^{i\alpha K_j|\vec{r}-\vec{r}'|} - 2\mu_0/m}{\alpha|\vec{r}-\vec{r}'|} \right], \tag{33}$$

where we have assumed the center of mass of the proton and the molecule to be initially at rest ($K \simeq 0$), and

$$K_j = \left[\frac{2\mu'}{\hbar^2}(E - E_j) \right]^{1/2} \tag{34}$$

and the ψ's are defined as before. Also

$$E_j = E_{n_1,n_2,n_3} = \frac{\hbar^2}{\mu_p} \sum_{i=1}^{3} (n_i + \tfrac{1}{2})/b_i^2 , \tag{35}$$

where μ_p is the reduced mass of the proton and the rest of the molecule

$$\mu_p = \frac{m(M-m)}{M}$$

and

$$i K_j \alpha = -\beta \left[2 \sum_{i=1}^{3} n_i/b_i \right]^{1/2} , \tag{36}$$

where

$$\beta = \left[\frac{M-m}{M+m} \right]^{1/2} .$$

Also,

$$q_i = \exp(-2\beta^2\tau/b_i^2) . \tag{37}$$

Carrying the sum over j, it is found[3,12]

$$\sum_{j=0}^{\infty} \Phi_j(\vec{r})\Phi_j^*(\vec{r}') \frac{2(\mu'/m)e^{iK_j\alpha|\vec{r}-\vec{r}'|} - 2\mu_0/m}{\alpha|\vec{r}-\vec{r}'|}$$
$$= \frac{1}{\alpha\sqrt{\pi}} \int_{\tau=0}^{\infty} \frac{d\tau}{\tau^{3/2}} \left[\frac{\mu'}{m} \prod_i \left\{ \exp\left[-\frac{1+q_i^2}{2(1-q_i^2)b_i^2} \left(\vec{r}_i^{\,2} + \vec{r}_i'^{\,2} - \frac{4q_i}{1+q_i^2} \vec{r}_i \vec{r}_i' \right) \right] \right\} \Big/ b_i\sqrt{\pi}(1-q_i^2)^{1/2} - \frac{\mu_0}{m}\delta(\vec{r}-\vec{r}') \right] . \tag{38}$$

Substituting (38) into (33) and carrying out the integrals we find[3,12]

$$T_{1fi} = -\frac{8\sqrt{\pi}\hbar^2 a^2}{\alpha m} \int_0^{\infty} d\tau \left[\frac{\mu'}{m} \prod_i [4\tau + 2b_i^2(1-q_i)]^{-1/2} - \frac{2\mu_0}{m}(16\tau^{3/2})^{-1} \right] . \tag{39}$$

From Eq. (39) it follows that the integral over τ appears to diverge in the region of small τ. To investigate the behavior of the integral in this region, we expand q_i in powers of τ and keep only the first two terms, i.e.,

$$q_i = 1 - \frac{2\tau\beta^2}{b_i^2} . \tag{40}$$

Representing the integrand in (39) by the symbol I we find that in the limit of $\tau \to 0$,

$$I \to \frac{\mu'}{m}[4\tau(1+\beta^2)]^{-3/2} - 2\frac{\mu_0}{m}(16\tau^{3/2})^{-1} . \tag{41}$$

In order for T_1 to converge, it is necessary that the coefficients of $\tau^{-3/2}$ in (41) be equal. This means

$$\mu_0 = \mu' \left[\frac{2\mu'}{m} \right]^{-3/2} . \tag{42}$$

From Eq. (42) we can derive the condition for the convergence or the first-order correction to the Fermi approximation when the mass of the binding molecule approaches infinity since $\lim_{M\to\infty}\mu' = m$,

$$\mu_0 = m\, 2^{-3/2} . \tag{43}$$

B. Ideal Gas

In this section we consider the case of an ideal gas, i.e., a single free nucleus with mass m_1 at position $\vec{r}_N$. We will derive the first-order correction to the Fermi approximation and discuss the conditions for the convergence of this term. For this system

$$\phi_j(\vec{r}) = e^{i\vec{q}_j\cdot\vec{r}} . \tag{44}$$

Substituting this into (18), we arrive at

$$T_{1fi}=\left[\frac{2\pi\hbar^2}{m}a\right]^2\sum_{jl}\int\int d^3r'\,d^3r\,e^{-i\vec{q}_f\cdot\vec{r}_N}e^{i(\vec{k}_l-\vec{k}')\cdot\vec{r}_N}$$
$$\times e^{i\vec{q}_j\cdot\vec{r}_N}e^{-i\vec{q}'_j\cdot\vec{r}'_N}e^{i\vec{q}_j\cdot\vec{r}'_N}e^{i(\vec{k}-\vec{k}_l)\cdot\vec{r}'_N}e^{i(\vec{k}-\vec{k}_l)\cdot\vec{r}'_N}(G_{jl}-G_{0l})\,, \tag{45}$$

where

$$G_{jl}=\left[E-E_j-\frac{\hbar^2k_l^2}{2m}+i\epsilon\right]^{-1} \tag{46}$$

and

$$G_{0l}=(-\hbar^2k_l^2/2\mu_0+i\epsilon)^{-1}\,. \tag{47}$$

Carrying out the integrals we find

$$T_{1fi}=\left[\frac{2\pi\hbar^2}{m}a\right]^2(2\pi)^6\sum_{jl}\delta(\vec{q}_j+\vec{k}_l-\vec{k}'+\vec{q}_f)\delta(\vec{q}_i+\vec{k}-\vec{k}_l-\vec{q}_j)(G_{jl}-G_{0l})\,. \tag{48}$$

Substituting

$$E_j=\hbar^2q_j^2/2m_1$$

and

$$\sum_l\rightarrow\frac{1}{(2\pi)^3}\int d^3k_l\,, \tag{49}$$

we arrive at

$$T_{1fi}=\left[\frac{2\pi\hbar^2}{m}a\right]^2(2\pi)^3\delta(\vec{q}_i-\vec{q}_f+\vec{k}-\vec{k}')$$
$$\times\sum_j\left[1\Big/\left[E-\frac{\hbar^2q_j^2}{2m_1}-\frac{\hbar^2}{2m}(\vec{q}_i+\vec{k}-\vec{q}_j)^2+i\epsilon\right]-1\Big/\left[-\frac{\hbar^2}{2\mu}(\vec{q}_i+\vec{k}-\vec{q}_j)^2+i\epsilon\right]\right]\,. \tag{50}$$

The sum over j can be carried out with the result

$$T_{1fi}=\left[\frac{2\pi\hbar^2}{m}a\right](-iKa)(2\pi)^3\delta(\vec{q}_i-\vec{q}_f+\vec{k}-\vec{k}')\,. \tag{51}$$

From Eq. (13) the matrix elements of the T matrix for an ideal-gas system are exactly given by

$$T_{fi}=\frac{2\pi\hbar^2}{m}a\frac{1}{1+iKa}(2\pi)^3\delta(\vec{q}_i-\vec{q}_f+\vec{k}-\vec{k}')\,, \tag{52}$$

and for T_0 from Eq. (14)

$$T_{0fi}=\frac{2\pi\hbar^2}{m}a(2\pi)^3\delta(\vec{q}_i-\vec{q}_f+\vec{k}-\vec{k}')\,. \tag{53}$$

Comparing Eqs. (51), (52), and (53) it is clear that T_{0fi} and T_{1fi} are the first and second terms in the expansion of T_{fi}:

$$T_{fi}=\frac{2\pi\hbar^2a}{m}(1-iKa+\ldots)(2\pi)^3\delta(\vec{q}_i-\vec{q}_f+\vec{k}-\vec{k}')\,. \tag{54}$$

C. Particle bound in a finite potential

Next, we move on to consider the case of neutron scattering from a nucleus bound in a finite potential. In this case the high-energy intermediate wave function of the scatterer are plane waves,

$$\phi_j(\vec{r})\rightarrow e^{i\vec{q}_j\cdot\vec{r}}\,. \tag{55}$$

The terms in the brackets $\langle\ \rangle$ in (18) are of the form

$$\int d^3r_N\phi_f(\vec{r}_N)e^{i(\vec{q}_j+\vec{k}_l-\vec{k}')\cdot\vec{r}_N} \tag{56}$$

and

$$\int d^3r_N\phi_i(\vec{r}_N)e^{i(\vec{k}-\vec{k}_l-\vec{q}_j)\cdot\vec{r}_N}\,.$$

These integrals approach zero at high values of q_j and k_l, unless

$$\vec{q}_j+\vec{k}_l=0\,. \tag{57}$$

Substituting this condition in (18) with

$$E_j=\frac{\hbar^2q_j^2}{2m_1}$$

$(G_{j1}-G_{01})$ becomes

$$\left[\frac{1}{E-\left[\frac{\hbar^2}{2m_1}+\frac{\hbar^2}{2m}\right]q_j^2+i\epsilon}-\frac{1}{-\frac{\hbar^2 q_j^2}{2\mu_0}+i\epsilon}\right] \tag{58}$$

which is equal to

$$\left[\frac{1}{E-\frac{\hbar^2 q_j^2}{2\mu}+i\epsilon}+\frac{1}{\frac{\hbar^2 q_j^2}{2\mu_0}+i\epsilon}\right] . \tag{59}$$

Therefore it is clear that the condition for convergence of the first-order correction to the Fermi approximation for neutron scattering from a nucleus bound in a finite potential is

$$\mu_0=\mu , \tag{60}$$

where μ is the reduced mass of the neutron and the scatterer

$$\mu=\frac{mm_1}{m+m_1} . \tag{61}$$

This choice causes Eq. (59) to go to zero at large values of q_j which are the values that can cause divergence and thus are those that we are concerned with.

The choice of a finite potential to represent the bound nucleus more realistically resembles the actual systems at high energies, since at higher energies the bound particle acquires sufficient energy so that its kinetic energy greatly exceeds the binding potential energy and the scatterer can be considered to be free.

V. COMPARISON WITH OTHER STUDIES

So far we have studied the first correction term to the Fermi approximation for three specific models. Our method is based on the expansion method described by Eq. (5) with the value of μ_0 chosen at our convenience, since the first term in that expansion, which is the Fermi approximation, is independent of μ_0.

We have studied thermal-neutron scattering from a particle bound in an infinitely heavy molecule by choosing a harmonic oscillator wave function to represent the bound scatterer. This is similar to the case considered by Breit and Zilsel[3] where they claimed that the first-order correction term converges. We found this to contradict our results which indicates that the first correction term diverges unless we choose $\mu_0=2^{-3/2}m$, with m being the mass of the neutron, as opposed to Breit and Zilsel's choice of $\mu_0=m/2$. In further reviewing their work it becomes clear that in going from their Eq. (3.1) to their (3.2), i.e., from, respectively,

$$\frac{1}{\pi^{1/2}}\int_0^\infty\left[\frac{\exp[-(\xi_\pi^2+\xi'^2)(1+q_x^2)/2(1-q_x^2)+2q_x\xi_\pi\xi'/(1-q_x^2)]}{\sqrt{\pi}\alpha_x(1-q_x^2)^{1/2}}-\frac{\delta(r_\pi-r')}{2}\right]\frac{\exp(-|r_\nu-r'|^2/4\tau)}{\tau^{3/2}}d\tau$$

to

$$\frac{8}{\pi^{1/2}}f(r_\pi)\int_0^\infty\left[\prod(4T_x)^{-1/2}\exp[-(x_\nu-q_x x_\pi)^2/4T_x]-\exp(-|r_\nu-r_\pi|^2/8\tau)/(8\tau)^{3/2}\right]d\tau$$

with

$$4T_x=4\tau+\alpha_x^2(1-q_x)^2 .$$

Their change of variable

$$\tau\rightarrow 2\tau$$

was only made in the second term in the integral (3.1). This led to the elimination of the divergent terms in the limit of $\tau\rightarrow 0$ and is clearly wrong.

In his work Ekstein[8] represented the bound proton in a highly excited state by a plane wave. His results indicate that the second term in the scattering matrix expansion always diverges unless the scatterer is attached to an infinitely heavy molecule. However, a plane-wave representation does not apply to a harmonic oscillator binding problem, since for the harmonic oscillator the average kinetic energy equals the average potential energy. Furthermore, a closer look at his calculations indicates that he has omitted the factor α in Eq. (31).

Next we consider Davydov and Mel'Nichenkov's[7] work. They concluded that the first correction to the Fermi approximation always diverges if the scatterer is bound by a harmonic oscillator wave function and it always converges if it is bound in a finite potential where high-energy states are represented by plane waves. Davydov and Mel'Nichenkov used for the harmonic oscillator

$$\mu_0=m/2 ,$$

and therefore they found divergent results for the first-order correction term to the Fermi approximation. They also used the same value for μ_0 when studying finite potentials and obtained convergent results for this case.

VI. MAGNITUDE OF THE CORRECTIONS

There have been several studies of the magnitude of the first-order correction to the Fermi approximation for scattering of slow neutrons from nuclei.[2-8] In all these studies the magnitude of the first-order correction has been calculated to be only a fraction of a percent. Breit,[2] who stated the problem of slow neutron scattering in terms of a boundary condition and its equivalent integral equation, calculated a first-order correction to the Fermi

approximation which he estimated to be 0.1%. Breit and Zilsel,[3] using a three-dimensional harmonic oscillator model, found the correction to be about 0.3% for zero-energy neutrons. Zilsel, Darling, and Breit[6] extended this work to neutron energies of 0.3 and 0.5 times the molecular level spacing and again found corrections of about 0.3%. Another study[5] extended the calculations to include neutron energies up to 15 times thermal energy. They found, again, the Fermi approximation to be accurate to within 0.3%.

In this study, after establishing new conditions for the convergence of the first correction term, it seemed desirable to conduct a numerical calculation of this term and to estimate its magnitude. However, after looking closer at the problem it is clear that such an undertaking is unnecessary. The general way of performing these numerical calculations is to replace the sum over the intermediate states of the scatterer by its first few terms, i.e., replacing the sum over j in (31) (with $M\rightarrow\infty$ and $\mu'\rightarrow m$) with the first one or two terms of the sum. To get an idea of the magnitude of each term on the right-hand side of (31) we substitute the sum over j by the first term, i.e., say the initial state ϕ_i. We also take the final state ϕ_f to be equal to the initial state. Since for thermal neutrons

$$e^{i\vec{k}\cdot\vec{r}}\simeq 1 ,$$

we substitute the two exponential terms by unity. Of the two terms in the bracket on the right-hand side of (31), only one need be considered; for simplicity, we take the second term. With these in mind the magnitude of the quantity associated with the second term in the brackets in (31) is given by

$$a\int\int d^3r\, d^3r'\phi_i^*(\vec{r})\phi_i(\vec{r}')\phi_i(\vec{r})\phi_i^*(\vec{r}')\frac{1}{|\vec{r}-\vec{r}'|} . \quad (62)$$

Substituting for the wave functions a harmonic oscillator, and carrying out the integrals, we find the magnitude of the corrections to be $\simeq 10^{-3}$. Therefore, a change in the second term caused by using

$$\mu_0 = m\,2^{-3/2} , \quad (63)$$

instead of the value used by others

$$\mu_0 = m/2 , \quad (64)$$

would not effect the order of magnitude of the correction resulting from the substraction of the two terms in Eq. (31). Therefore we agree with the previous studies insofar as the magnitude of the first-order correction is concerned.

VII. CONCLUSIONS

From the results of this study it may be concluded that a zero-range potential approach can be taken to develop a consistent method of dealing with the first-order correction to the Fermi approximation which will lead to convergent results for this term for all systems. Our approach has been based on the substitution of the scattering nucleus by a boundary condition, which leads to the replacement of the Fermi pseudopotential by a new pseudopotential to describe the interaction, and the use of an expansion for the scattering matrix other than the Born series.

The results indicate that by the consistent application of this method, convergent results can always be obtained for the first-order correction to the Fermi approximation. Furthermore, they confirm previous results that indicate the corrections are small.

ACKNOWLEDGMENTS

This work was supported in part by the National Science Foundation Grant No. DMR-79-26254.

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