Validity of the Fermi Approximation in Slow Neutron Scattering*

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(Received 21 February 1963)

The correction to the Fermi approximation for the cross section is calculated for slow neutron scattering from a proton bound in a harmonic potential. For neutron energies up to fifteen times thermal energy, and for energy transfer due to proton transitions between the ground state and first excited state, the Fermi approximation is found to be accurate to 0.3%. This extends previous calculations, which have been done for $d\sigma/d\Omega$, and which considered only elastic scattering from the proton initially in the ground state. This extension is believed to be necessary, because of the extensive use that is made of the Fermi approximation to calculate the energy distribution of scattered neutrons.

I. INTRODUCTION

THE scattering of low-energy neutrons is commonly treated by the Fermi approximation.[1] Breit[2] stated the problem of slow neutron scattering from a target nucleus bound in a molecule in terms of a boundary condition and its equivalent integral equation. He 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 that the correction to the Fermi approximation is about 0.3% for zero-energy neutrons. Breit, Zilsel, and Darling[4] 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%.

Lippman and Schwinger[5] applied a variational technique to derive the first-order correction to the Fermi approximation. Using these results, Lippmann[6] calculated a 0.3% correction to the Fermi approximation for zero energy neutron scattering from parahydrogen.

Thus, the Fermi approximation has not been checked for neutron energies sufficient to excite the molecule, or for the molecule initially in an excited state. Since the Fermi approximation is frequently used to give results for these cases, we extend the calculations to consider neutron scattering from a harmonically bound proton for neutron energies sufficient to excite the molecule, and for the molecule initially in an excited state.[7] However, we only consider a single scattering nucleus.

II. CALCULATION

The following expression gives the differential scattering cross section.

$$\frac{d\sigma_{fi}}{d\Omega}=\left(\frac{M}{2\pi\hbar^2}\right)^2\frac{k_f}{k_i}|T_{fi}|^2, \tag{1}$$

M is the neutron mass; $\mathbf{k}_f$ and $\mathbf{k}_i$ are, respectively, the final and initial neutron wave vectors. The matrix element, T_{fi}, for a single target proton is approximated as follows in Ref. 5.

$$T_{fi}\simeq-\frac{4\pi\hbar^2}{M}a\Bigg\{\int\exp(-i\mathbf{k}_f\cdot\mathbf{r})\chi_f^*(\mathbf{r})\chi_i(\mathbf{r})\exp[i\mathbf{k}_i\cdot\mathbf{r}]d^3r$$
$$+a\sum_\gamma\int\exp(-i\mathbf{k}_f\cdot\mathbf{r})\chi_f^*(\mathbf{r})\chi_\gamma(\mathbf{r})$$
$$\times\frac{(2\mu/M)\exp(ik_\gamma|\mathbf{r}-\mathbf{r}'|)-1}{|\mathbf{r}-\mathbf{r}'|}\chi_\gamma^*(\mathbf{r}')$$
$$\times\chi_i(\mathbf{r}')\exp(i\mathbf{k}_i\cdot\mathbf{r}')d^3rd^3r'\Bigg\}. \tag{2}$$

The first term in Eq. (2) is the Fermi approximation; the second term is the first-order correction; the indices "i" and "f" denote initial and final states, respectively; "a" is the free atom scattering length; χ_n is the bound proton wave function for the nth state; and μ is the reduced mass of the neutron and the molecule. The wave number, k_γ, is given by

$$k_\gamma=\left\{\frac{2\mu}{\hbar^2}(E-W_\gamma)\right\}^{1/2};\quad W_\gamma<E.$$
$$=i\left\{\frac{2\mu}{\hbar^2}(W_\gamma-E)\right\}^{1/2};\quad W_\gamma>E. \tag{3}$$

E is the initial energy of the entire system; and W_γ is the energy of the γth molecular state.

The wave functions of the proton, χ_γ, were determined by assuming the proton was bound to an infinite mass by a harmonic potential, and taking $l=0$. The resultant wave functions are

$$\chi_n(r)=\frac{1}{2\sqrt{\pi}}(\pi^{1/2}2^n n!X_0)^{-1/2}$$
$$\times H_n\left(\frac{r}{X_0}\right)\frac{\exp(-r^2/2X_0^2)}{r}, \tag{4}$$

* Work supported by the U. S. Atomic Energy Commission, Contract No. AT(11-1)-917.

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[5] B. A. Lippmann and Julian Schwinger, Phys. Rev. **79**, 469 (1950).
[6] B. A. Lippman, Phys. Rev. **79**, 481 (1950).
[7] The need for such an extension has been pointed out by M. Nelkin, in *International Atomic Energy Agency Symposium on Inelastic Scattering of Neutrons in Solids and Liquids Vienna, 1961* (International Atomic Energy Agency, Vienna, 1961).

where H_n is the Hermite polynomial of order n; and X_0 is given by

$$X_0=(\hbar/M\omega)^{1/2}.$$

The energy levels are given by

$$W_n=(2n+3/2)\hbar\omega;\quad n=0,1,2,\cdots. \tag{5}$$

The level spacing was chosen to be 0.27 eV. This corresponds to the level spacing in ZrH, which is found to agree closely with a harmonic oscillator model.[8] The scattering length was taken to be the singlet neutron-proton scattering length, $a=-2.4\times10^{-12}$ cm.

T_{fi} was calculated numerically from Eq. (2) for three values of the incident neutron energy—0.025, 0.27, and 0.405 eV—and for the proton in the ground state and first excited state. We eliminated the divergence problems discussed by Davydov and Mel'nichenko[9] and Ekstein[10] by terminating the sum on γ in Eq. (2) at the third excited state. This procedure is reasonable, since a physical molecule is not well represented by a harmonic oscillator model at high energies. For further discussion of this point, see Ref. 9. The cross sections in the Fermi approximation and the percent difference given by the correction in Eq. (2) are shown in Table I. The results are given for each incident energy and for the possible molecular transitions between the ground state and first excited state. In every case considered, the correction to the Fermi approximation is 0.3% or less.

III. DISCUSSION

We have shown that the Fermi approximation is accurate to 0.3% for incident energies up to 0.405 eV, for scattering from a single nucleus bound by a harmonic potential. In particular, we have shown this for processes in which energy is transferred due to transitions of the proton between the ground state and the first excited state. This extends previous results, in which the Fermi approximation has been shown to be valid for elastic scattering and incident energies up to 0.12 eV. This extension is felt to be important in view of the extensive use that is made of the Fermi approximation to calculate the energy distribution of neutrons scattered by a moderator.

Unfortunately, the expression for the correction to the Fermi approximation is so complicated that there is no simple way to determine, even qualitatively, how the magnitude of the correction might be expected to vary with changes in the degree of binding, level spacing, etc., of the scattering system. However, the numerical results presented here lead one to believe that such changes would be small. It would seem that the primary mechanism for increasing the corrections calculated in Refs. 2–6 would be the possibility of energetically allowed intermediate states. This possibility is shown to have little if any effect on the corrections, cf. Table I.

There is still a further extension that is necessary. The correction to the Fermi approximation has not been calculated for scattering systems with more than two nuclei. Since the Fermi approximation does not give multiple scattering effects, it is clear that it is not valid for systems whose dimensions are on the order of a neutron mean free path. It is not clear how such multiple scattering corrections enter the expression for the cross section.[11] It would be instructive to calculate the relative importance of collective excitations (i.e., a process in which two nuclei are excited, described by the Fermi approximation), and multiple scattering excitations (i.e., a process in which two nuclei are excited described by the first-order correction to the Fermi approximation).

TABLE I. σ_{fi} (in b) for neutron scattering from a proton bound by a harmonic potential.[a]

p Incident neutron energy	σ_{00} Ground state to ground state	σ_{10} Ground state to first excited state	σ_{01} First excited state to ground state	σ_{11} First excited state to first excited state
0.0926	64.8(0.3%)	0(0)	43.2(<0.1%)	52.0(<0.1%)
1.0	66.4(0.1%)	0(0)	14.7(<0.1%)	18.9(<0.1%)
1.5	29.6(0.2%)	6.28(<0.1%)	13.3(<0.1%)	18.1(<0.1%)

[a] The subscripts on the cross sections refer to the index n in Eqs. (4) and (5). The incident neutron energy is expressed in units of the level spacing, $E_0=2p\hbar\omega=0.27\times p$ eV. The cross section in the Fermi approximation and the percent correction are listed for each energy and transition.

ACKNOWLEDGMENTS

We wish to express our gratitude to Professor P. F. Zweifel for numerous illuminating discussions and suggestions. We also wish to thank the University of Michigan computing center for the use of their facilities. One of us (JPP) thanks Jon Erickson for assistance with the numerical work.

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