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Role of an Electron Screened Mott–Schwinger Interaction in the Elastic Scattering of Neutrons

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Abstract

The Mott–Schwinger potential arising from the interaction of the magnetic moment of a neutron incident upon the (electric) field of a nucleus has a profound effect upon the cross sections for scattering. The purely nuclear interaction (hadronic plus Mott–Schwinger) leads to a divergence in the spin–flip scattering amplitude at 0° scattering and thus to a divergent total scattering cross section. We demonstrate that the screening of this interaction caused by the atomic electron cloud essentially compensates that divergence so that the scattering cross-section values, to be used for example in reactor moderation calculations, are effectively those given by calculations made without consideration of any Mott–Schwinger potential. However, the forward scattered neutrons remain strongly polarised as a result of the (complete) Mott–Schwinger interaction.

1. Introduction

The cross sections for neutron–nucleus scattering are important in the evaluation of how neutrons slow in their passage through matter. Such information is needed to understand the details of how neutrons are detected, as well as what is needed to moderate and thermalise them in reactors. To date those cross sections have been evaluated by use of an optical model potential scattering theory wherein the optical potential is chosen phenomenologically. That optical potential usually is taken to be of local form having both a central and a spin–orbit character. Woods–Saxon form factors for those fields are chosen most often, so that the potential is short range and decreases exponentially, reflecting the characteristic of the underlying two nucleon (NN) g matrices.

The Mott–Schwinger (MS) interaction is electromagnetic in origin, arising specifically from the interaction between the (moving) magnetic moment of the neutron and the electric field of the target. The result, a spin–orbit term in the Schrödinger interaction for the system, is relatively weak in strength (compared to that of the nuclear field) but has very long range. Specifically the nuclear MS interaction varies as r^{-3}. Previous studies (Mott 1929; Schwinger 1948; Sample 1956; Monahan and Elwyn 1964; Hogan and Seyler 1969; Eriksson 1957; Alexander *et al.* 1994) have shown that this MS interaction can have a marked effect upon nucleon scattering observables at small angles and at all energies (to 130 MeV). But the most dramatic effects occur for low energy neutrons incident upon heavy targets. Even so, the differences in cross

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sections and polarisations caused by the nuclear MS effect are limited to very small scattering angles; scattering angles that are usually not included in experimental studies. Nevertheless, the total scattering cross sections being integrals over all scattering angles of the differential cross sections will reflect the variations provided that they are large enough. That is certainly the case with the bare nuclear field MS effect as the variation caused to the nuclear cross section at 0° diverges as $\cot^2(\theta/2)$.

Many previous calculations of the MS effect did not take into account the contribution due to the electric field screening caused by the atomic electrons. But Shull and Ferrier (1963) observed the effect of the MS interaction in the scattering of slow neutrons from a single crystal of pure vanadium for which Shull (1963) demonstrated electron screening needed to be included in the analysis to match observation. In Shull's analysis, and in the discussion of that effect in a recent text on neutron interactions with matter (Byrne 1994), the screening to offset the divergence in scattering amplitudes found by considering the purely nuclear (MS) interaction is introduced as a scaling factor of the form $(1-f_e(q))$ on the spin–flip scattering amplitude. With q being the momentum transfer in the (elastic) scattering process, this factor vanishes in the limit $\theta \to 0$ as then $q \to 0$ and $f_e(q) \to 1$. Thereby the neutron cross sections remain finite and, to a good approximation, equal to the purely nuclear (hadronic interaction) values. As we will demonstrate, that is also the case when the electron screening is included as a (compensating) electric field in the interaction Hamiltonian and numerical solutions of the neutron–atom Schrödinger equations found. In particular, we present an analysis of the differential cross sections, the polarisations and the total cross sections for neutron scattering from ^{209}Bi and for energies ranging from $0 \cdot 01$ to $14 \cdot 5$ MeV. The results are compared with ones obtained by using the method of Shull (1963). In the latter calculations, the scaling form factor was taken to be the Fourier transform of the model charge density used in our 'exact' calculations. The 'exact' and Shull method results are virtually indistinguishable.

Details of the MS interaction form used and its role in scattering calculations are given next. The results are presented in Section 3 and conclusions that can be drawn follow in Section 4.

2. MS Interaction for Neutron–Atom Scattering

Assuming that the process is effected by a nuclear (hadronic) interaction modified by a MS interaction, we seek solutions to the Schrödinger equations containing potentials of the form

$$\begin{aligned} V_{nucl+MS}(r) = &-V_0 f(r, r_0, a_0) - iW_0 f(r, r_w, a_w) - i\ 4a_d W_d f'(r, r_d, a_d) \\ &+ (V_{so} + iW_{so})\left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r} f'(r, r_{so}, a_{so}) \\ &+ \zeta(r)\frac{\mathbf{L}\cdot\mathbf{s}}{r^3}\,, \end{aligned} \tag{1}$$

and where, with $\zeta_0 = \mu_n Z e^2 \hbar^2 / m^2 c^2$,

$$\zeta(r) = \begin{cases} \zeta_0 \frac{1}{Z} Z(r) & \text{if } r \geq R_{Nucl} \\ \zeta_0 r^3 / R_{Nucl}^3 & \text{if } r < R_{Nucl}\,. \end{cases} \tag{2}$$

Thus, inside the nuclear radius, the MS interaction is taken to be a constant. The absorption terms are relevant if the projectile energy lies above the first reaction threshold. The form factors, $f(r, r_x, a_x)$, usually are taken to be of Woods–Saxon type and these have been used herein for the neutron scatterings from ^{209}Bi of interest. The parameter values used in our calculations are those given previously (Hogan and Seyler 1969).

Solution of the Schrödinger equation gives the scattering amplitudes

$$f_{\nu,\mu}(\theta) = g(\theta)\delta_{\nu,\mu} + h(\theta)\langle\sigma \cdot \hat{\mathbf{n}}\rangle_{\nu,\mu} \,. \tag{3}$$

The measurables are given by

$$\frac{d\sigma}{d\Omega} = |g(\theta)|^2 + |h(\theta)|^2 \tag{4}$$

for the differential cross section, by

$$P(\theta) = \frac{2\Re(g^*(\theta)h(\theta))}{d\sigma/d\Omega} \tag{5}$$

for the polarisation (the x–z plane is taken as the scattering plane) and, by angular integration of the differential cross section,

$$\sigma_{tot}(E) = \int |g(\theta)|^2 d\Omega + \int |h(\theta)|^2 d\Omega \,, \tag{6}$$

one finds the total (elastic) scattering cross section.

It is customary to use partial wave expansions whence all measurables are specified in terms of phase shifts, $\delta_\ell^{(\pm)}$, wherein the superscripts designate $j = \ell \pm \frac{1}{2}$, and we find

$$g(\theta) = \frac{1}{2ik}\sum_{\ell=0}^{\infty}\left[(\ell+1)e^{2i\delta_\ell^{(+)}} + \ell e^{2i\delta_\ell^{(-)}} - (2\ell+1)\right]P_\ell(\theta)\,, \tag{7}$$

$$h(\theta) = \frac{1}{2k}\sum_{\ell=1}^{\infty}\left[e^{2i\delta_\ell^{(+)}} - e^{2i\delta_\ell^{(-)}}\right] P_\ell^1(\theta)\,. \tag{8}$$

The total cross section then is given by

$$\begin{aligned}\sigma_{tot} &= \frac{\pi}{k^2}\left[\sum_{\ell=0}^{\infty}\frac{1}{2\ell+1}\left((\ell+1)e^{2i\delta_\ell^{(+)}} + \ell e^{2i\delta_\ell^{(-)}} - (2\ell+1)\right)^2\right.\\ &\qquad\left. + \sum_{\ell=1}^{\infty}\frac{\ell(\ell+1)}{(2\ell+1)}\left(e^{2i\delta_\ell^{(+)}} - e^{2i\delta_\ell^{(-)}}\right)^2\right]\\ &= \frac{\pi}{k^2}(G_{sum} + H_{sum})\,.\end{aligned} \tag{9}$$

For the cases of interest, $0{\cdot}01$ to $14{\cdot}5$ MeV neutrons scattered from ^{209}Bi, and considering only the hadronic interaction (no MS interaction at all), the infinite sums can be truncated to ℓ_{max} where $\ell_{max} \sim 20$ suffices. As has been shown (Alexander *et al.* 1994), when the nuclear MS effect ($Z(r) \to Z$) alone is considered, then all partial waves need be taken in the sums for the spin–flip amplitudes, $h(\theta)$, to have convergence. But for most partial waves, only the MS interaction has any effect and for them ($\ell > \ell_{max}$) the Born approximation is very good. One need only evaluate numerically the actual partial wave phase shifts for $\ell \leq \ell_{max}$ and then use the Born approximation results for the remainder. Those Born approximation phase shifts are analytic and are specified by

$$\sin(\delta_\ell^+) = -\frac{mk\zeta_0}{2\hbar^2(\ell+1)}, \tag{10}$$

$$\sin(\delta_\ell^-) = \frac{mk\zeta_0}{2\hbar^2\ell}. \tag{11}$$

With these phase shifts the scale factors, G_{sum} and H_{sum}, in the total cross-section functions tend with increasing ℓ as

$$\frac{1}{2\ell+1}\left((\ell+1)e^{2i\delta_\ell^{(+)}} + \ell e^{2i\delta_\ell^{(-)}} - (2\ell+1)\right)^2 \to 0, \tag{12}$$

$$\frac{\ell(\ell+1)}{(2\ell+1)}\left(e^{2i\delta_\ell^{(+)}} - e^{2i\delta_\ell^{(-)}}\right)^2 \to \left(-\frac{imk\zeta_0}{\hbar^2}\right)^2 \frac{(2\ell+1)}{\ell(\ell+1)}, \tag{13}$$

respectively. Thus while the summation for G_{sum} converges rapidly and can be truncated, that of the spin–flip component tends as

$$H_{sum} \to \sum \frac{(2l+1)}{l(l+1)}; \tag{14}$$

an infinite sum that diverges logarithmically. That divergence is also apparent from the optical theorem by which the total cross section relates to the imaginary parts of the forward scattering amplitudes. Thus, as the spin–flip amplitude $h(\theta)$ tends as $i\cot(\frac{1}{2}\theta)$ at small scattering angles, the total cross section diverges. We note that a similar problem arises with the Coulomb interaction, and an evaluation of the total cross section for proton scattering from nuclei must also take into account the atomic electron screening to circumvent a divergence in theory.

To allow for electron screening, we adopt a radial dependence for the charge distribution in the MS interaction. Specifically we consider $Z(r)$ to be the charge enclosed in a sphere of radius R centred upon the nucleus, viz.

$$Z(R) = Z - 4\pi \int_0^R \rho(r)\, r^2\, dr, \tag{15}$$

and we choose

$$\rho(r) = \frac{2k^2 Z}{4\pi}\, r\, e^{-kr^2}\,, \tag{16}$$

as then the charge distribution function is analytic, i.e.

$$Z(r) = Z(1 + kr^2)e^{-kr^2}\,. \tag{17}$$

Therewith the parameter k relates to the position where the maximum radius of the electron charge distribution occurs by

$$k = \frac{1}{2R_{max}^2}\,. \tag{18}$$

The reason for choosing an analytic form for $\rho(r)$ is to obtain an analytic expression for $Z(r)$, otherwise a more accurate measure would involve the radial wavefunctions of the atomic electrons via the probability

$$P(r)dr \propto R_{nl}^* R_{nl} r^2 dr\,. \tag{19}$$

However, as the total cross section is not sensitive to the exact choice of the charge density, it is convenient to use the model form. For ^{209}Bi approximately six principal quantum shells are filled, so that R_{max} can be estimated to be the Bohr orbit for the $n = 2$ or $n = 3$ state, and as

$$R_{max} = \frac{n^2 a_0}{Z}\,, \tag{20}$$

the appropriate values for $n = 2$ and $n = 3$ are 3000 and 5000 fm respectively, so giving choices for the parameter k.

But radial variation of the MS interaction now precludes use of an analytic form for large partial wave phase shifts. Albeit, the sums defining both $g(\theta)$ and $h(\theta)$ now converge without the necessity of taking the infinite sum, the interaction field is very long range (by nuclear standards) and ℓ_{max} for the evaluations will be extremely large. We have evaluated the results by the direct means nevertheless. In those numerical solutions of the partial wave Schrödinger equations, the parameter values of the phenomenological (hadronic) optical potential again were taken to be those used by Hogan and Seyler (1969). Scattering results found with that optical potential alone are compared with those obtained by using both the purely nuclear MS and the complete atomic MS interactions in addition. We have solved the partial wave Schrödinger equations numerically for partial waves $\ell \leq \ell_{max}$. With the pure optical potential calculations and with the nuclear MS additional interaction, the calculations were made for $\ell_{max} = 20$ and the analytic Born values for the larger-ℓ phase shifts were used. But for the electron screened cases, numerical integrations were made out to 10 000 fm and l_{max} was taken such that the larger-ℓ phase shifts had a magnitude of order 10^{-10}. With the electron screening, eventually the partial wave phase shifts rapidly decrease to zero. Such occurs for

$$\ell \sim kb\,, \tag{21}$$

where b is the impact parameter at which the charge distribution can be taken as zero. Our charge sphere extends to 10,000 fm and therefore, when $l_{max} > 10000k$, the partial wave function is essentially a Bessel function. We checked that to be the case numerically.

We have also checked the results of our 'exact' numerical evaluations with those found by using the method of Shull (1963) in which the spin-flip amplitude is taken to have the form

$$h(\theta) = h_{nucl}(\theta) - i\frac{Ze^2\mu_n}{2mc^2}\left[1 - f_e(q)\right]\ \cot(\tfrac{1}{2}\theta)\,. \tag{22}$$

Therein, $h_{nucl}(\theta)$ is the spin-flip amplitude evaluated using only the hadronic nuclear interaction and $f_e(q)$ is the Fourier transform of the electron charge density distribution. The Fourier transform of the model charge density given in (16) is

$$\begin{aligned} f_e(q) &= \tfrac{1}{2}\ -\ \left(\frac{q}{2\sqrt{k'}} - \frac{\sqrt{k'}}{q}\right)\int_0^{q/2\sqrt{k'}} e^{(r^2-q^2/4k')}dr \\ &\underset{q\to 0}{\longrightarrow} 1\,. \end{aligned} \tag{23}$$

Comparisons have been made of the differential cross sections and polarisations for the scattering of 0·01, 0·5 and 14·5 MeV neutrons scattered from ^{209}Bi.

3. Results and Discussion

In the extensive electron screened calculations, the phase shifts were evaluated in steps of 10 from 10 to l_{max} and the intermediate results obtained by cubic splining those grid points, while the 0–9 phase shifts were evaluated individually. All summations to form total cross sections then were tested for convergence to 1 part in 10^7. The total cross sections for elastic scattering of neutrons with energies in the range 0·01 to 14·5 MeV are listed in Table 1. They are compared with the results found by purely nuclear (no MS) effects. In the complete calculations,

Table 1. Calculated total elastic cross sections for neutrons scattering from ^{209}Bi in the energy range 0·01 to 14·5 MeV

The results of calculations made using no MS interaction (purely nuclear optical potential) are compared with those found from the complete (MS from electron screening) calculations with the latter shown in parentheses. The components in the summation in equation (9), G_{sum} and H_{sum}, are also given

E (MeV)	G_{sum}	H_{sum}	σ_{tot}
0·01	0·1512440E+00	0·1566910E-08	0·1002630E+04
	(0·151244E+00)	(0·224342E-03)	(0·100412E+04)
0·50	0·7206760E+00	0·1143540E-06	0·9555040+03
	(0·720673E+00)	(0·131036E-02)	(0·957236E+03)
14·5	0·838343E+02	0·553922E+01	0·408605E+03
	(0·846252E+02)	(0·562490E+01)	(0·412612E+03)

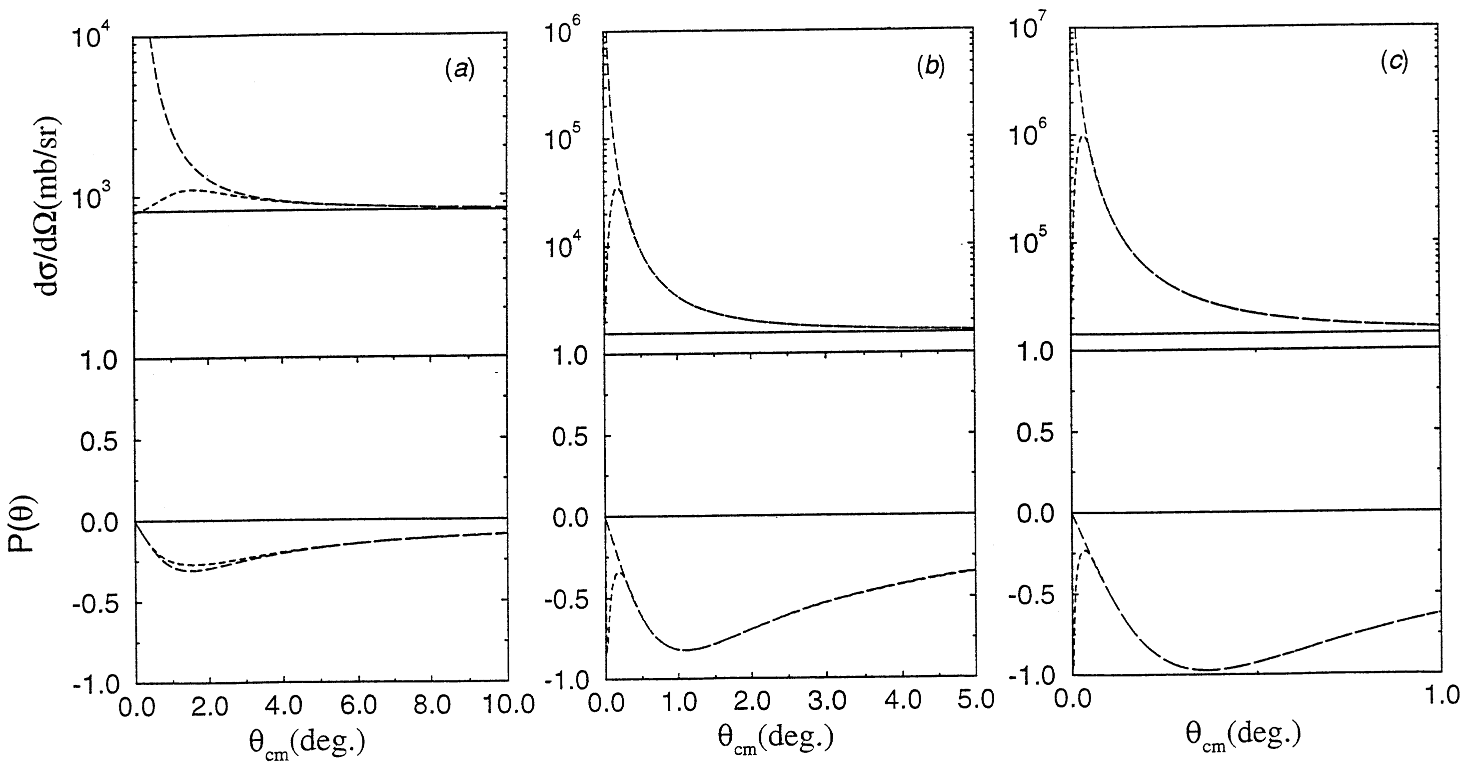

Fig. 1. Differential cross sections (top) and polarisations (bottom) for the elastic scattering of (*a*) 0·01 MeV, (*b*) 0·5 MeV and (*c*) 14·5 MeV neutrons from ^{209}Bi and for scattering angles at which the Mott–Schwinger interactions have noticeable effect. The solid curves portray the results found using the purely hadronic (nuclear) interaction in the Schrödinger equations. The long dashed curves represent the results found when the purely nuclear Mott–Schwinger contribution is included with the strong short ranged nuclear interaction in the calculations, and the short dashed curves are the results obtained with electron screening also included.

the electron probability maximum was taken at $R_{max} = 5000$ fm. Due to the (complete) MS interaction, the total scattering cross section is varied by at most 4 parts in 1000. Analysis of the separate component summations shows that, at the lower energies, inclusion of the the fully screened MS interaction in calculations has practically no effect on the non-spin-flip component but has a marked effect on the spin-flip one. However, as the overall magnitude of the non-spin-flip component for the lower energy scattered neutrons is still three orders of magnitude greater than the spin-flip one, it dominates the summation that forms the total cross section. A more significant increase in the total cross section is found with the scattering of 14·5 MeV neutrons. This is expected because higher energy scattered neutrons have many more partial wave states affected by the atomic field (≈10,000), than for the lower energy neutrons. That is evident from the results shown as the total cross sections are the areas under the low angle peaks of the differential cross sections, displayed by the short dashed curves in Fig. 1. Therein it is seen that the 14·5 MeV neutron results have a peak in the differential cross section two orders of magnitude greater than that expected from a nuclear only (no MS) interaction.

To test the sensitivity of the calculations to the specific charge distribution, total cross sections were calculated for the 0·05 MeV case using two values of R_{max}. The results are given in Table 2, from which it is evident that there is a very small variation in total cross section caused by the chosen value of R_{max}.

Table 2. Total elastic scattering cross section for 0·05 MeV neutrons from ^{209}Bi, evaluated using two different model charge distributions of the atomic electrons

	$R_{max} = 3000$ fm	$R_{max} = 5000$ fm
$\rho(r) \propto re^{-kr^2}$	0·957052E+03	0·957236E+03

These results demonstrate that, while electron screening has offset the divergence (at 0°) created by the purely nuclear field MS interaction, the total MS effect remains distinct and retains a signature in the differential cross sections and polarisations. Those effects are displayed in Fig. 1 for incident energies of 0·01, 0·5 and 14·5 MeV respectively. Only very forward angle results are shown as the MS effect has negligible effect elsewhere. The differential cross sections are given in the top section of each figure, while the polarisations are shown in the bottom section with the purely nuclear interaction results displayed by the solid curves. The results found allowing only for the nuclear MS effect are displayed by the long dashed curves and the complete (screened MS) results are shown by the short dashed curves. In the complete calculations, the phase shifts were generated using an electron screened MS interaction based on the charge density of equation (16) with R_{max} of 5000 fm.

The divergence of the differential cross section due to use of the purely nuclear MS interaction is evident in all cases. Associated with those cross sections, the polarisations vary markedly to almost total polarisation at a value θ_{crit} at the largest energy. As the energy decreases, however, so also does the degree of polarisation to have a peak at ~ 30% at 10 keV. The variation of those results was also understood (Alexander, *et al.* 1994) by means of a small angle expansion of the

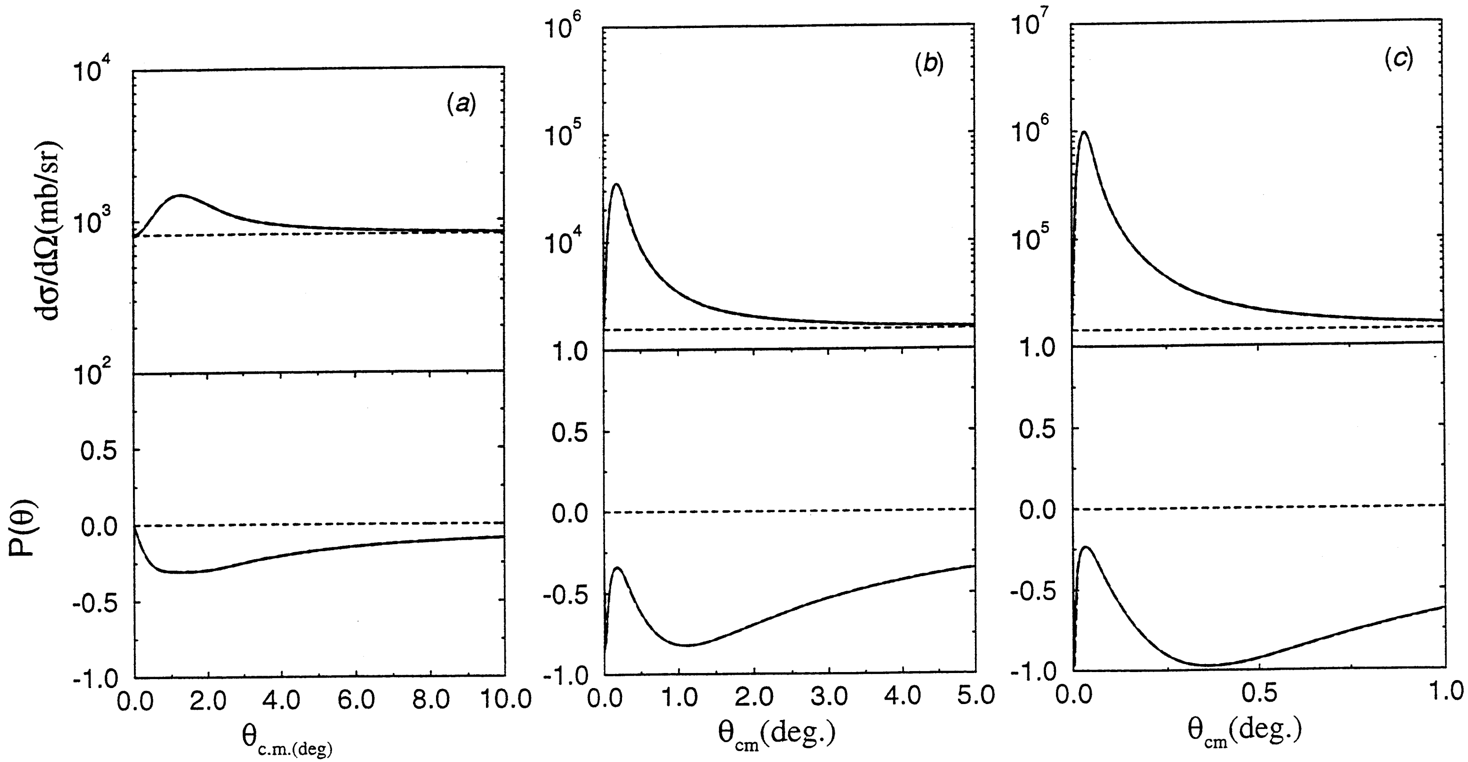

Fig. 2. Differential cross sections (top) and polarisations (bottom) for the elastic scattering of (*a*) 0·01 MeV, (*b*) 0·5 MeV and (*c*) 14·5 MeV neutrons from ^{209}Bi and for scattering angles at which the MS interactions have noticeable effect. The short dashed lines portray the results found using the purely hadronic (nuclear) interaction in the Schrödinger equations. The solid curves represent those obtained with electron screening in our 'exact' calculations. These overlap almost exactly the long dashed curves which display the results found by using the electron form factor correction to the scattering amplitude as prescribed by Shull (1963).

scattering amplitudes. When the electron screening is taken into account, the cross sections and polarisations follow the trends of the purely nuclear MS results as one moves from the larger angles (of the small angle sets displayed), but at the smallest angles there are departures in both observables from the previous results. The cross sections all have maxima and reduce to the purely hadronic value at 0° scattering. Those maxima are two orders of magnitude larger than the purely hadronic potential calculation results at 14·5 MeV, but the enhancement decreases as the energy is lowered to be less than a factor of 2 at 10 keV. Also those peaks are quite narrow and so the effect upon the total (elastic) scattering cross sections is small (2 parts in a 1000). The polarisations now have a double peak structure, again with the polarisation almost being total in the 14·5 MeV case. But that also reduces as the energy decreases. The extra structure in these results above that observed using the purely nuclear MS interaction coincides with the angles at which the differential cross sections have their maxima. It should be noted though that the MS effect upon the polarisation is evident to larger angles than it is in the associated differential cross section. Indeed for the case of 0·5 MeV neutron scattering, the polarisation remains $\geq -50\%$ for angles to 3° and for the case of 0·01 MeV it exceeds -20% to 5°. Finally, in Fig. 2, we present comparisons of the results obtained by using the method prescribed by Shull (1963) with those evaluated by direct numerical solution of the Schrödinger equations containing the complete nuclear plus MS interactions. Therein the differential cross sections and polarisations from the scattering of neutrons from ^{209}Bi are displayed for energies of 0·01, 0·5 and 14·5 MeV respectively. The short dashed lines portray the results found using the purely nuclear (no MS) interaction, the long dashed curves display the 'exact' results, while the solid curves portray those from the Shull method calculations. The latter two are in such excellent agreement over all energies and angles that differences are not apparent in the figures.

4. Conclusions

Electron screening of the nucleus has been shown to be very important in an accurate determination of the effect of the Mott–Schwinger interaction for neutrons incident upon matter. In particular, the divergence of both the total (elastic) cross sections and the 0° differential cross sections caused by the purely nuclear MS interaction were ameliorated and markedly so. The net effect of the complete MS calculations is that the total (elastic) cross sections vary little from those generated by the hadronic (purely nuclear) interaction of the neutron with the target nucleus. The complete Mott–Schwinger interaction (allowing electron screening) gave a marked variation in the small scattering angle differential cross sections and polarisations nevertheless, and that polarisation is very large. Forward scattering of neutrons through matter, via the MS interactions, may still be a means to polarise emergent neutrons. Finally, the model specification of Shull has been shown to be an excellent representation of the exact, calculated results.

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