Calculation of the interaction of a neutron spin with an atomic electric field

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The Thomas-Fermi approximation for an atomic wavefunction is used to calculate the interaction of a neutron spin with the atomic electric field, either through the motional magnetic ($\vec{v} \times \vec{E}$) or possibly electric (due to the possible existence of a neutron permanent electric dipole moment) couplings.

I. INTRODUCTION

Most recent experiments to search for the neutron electric dipole moment (EDM) involve the neutron interacting with electric fields created by laboratory apparatus. However there is also the possibility of using electric fields produced by atoms in crystals. There are some reasons for believing this might be advantageous – atomic fields are large and the neutrons interact with many atoms in a coherent fashion. However as we will show the measurable effects are quite small compared to known background effects due to the motional electric field.

The effect in a crystal experiment can be enhanced if the scattering amplitude due to the EDM interaction can be made to interfere with the much larger scattering amplitude of a nucleus. It will be seen below that the scattering amplitude due to the EDM interaction is imaginary so it can only interfere with an imaginary nuclear amplitude. The idea of searching for a neutron EDM by measuring the interference between the scattering from an atomic electric field (due to the EDM interaction) with nuclear scattering was proposed by Shull; an experiment was performed in 1964 and was based on scattering from a CdS crystal, because Cd, a strong absorber, has a large imaginary scattering amplitude. In this experiment, the penetration depth, hence reflectivity, depends on the orientation of the neutron spin relative to the momentum transfer.

Recently, a proposal to search for a neutron EDM by scattering in a perfect Si crystal was put forward. In this case, the imaginary part of the nuclear scattering length is very small, and the proposed observable is a rotation of the neutron spin direction caused by the superposition of the spin dependent imaginary amplitude with the real nuclear amplitude.

Because the calculations regarding this effect do not, to our knowledge, appear in the literature and the calculations regarding the Schull experiment are lacking in detail, we felt it worthwhile to estimate the size of a neutron spin rotation due to an EDM interaction, and in addition, include the analysis of the $\vec{v} \times \vec{E}$ interaction originally studied by Schwinger and demonstrated by Shull and Nathans. We use the Thomas-Fermi model of the atom to give the approximate atomic electric field.

II. THOMAS-FERMI MODEL OF THE ATOM

The Thomas-Fermi model of the atom is fully developed in §70 of \cite{7}. Briefly, the atom is treated semiclassically with the electron density as a function of position determined by phase space considerations. This leads to a universal function (i.e., it does not depend on atomic number $Z$) for the self-consistent electric field within the atom,

$$\sqrt{x} \frac{d^2}{dx^2} \chi = \chi^{3/2} \quad (1)$$

where $\chi$ describes the shielding (assumed spherically symmetric) of the nuclear point charge, with the boundary conditions that $\chi(0) = 1$ and $\chi(\infty) = 0$ (the latter condition determines $\chi'(0)$), and the radius $r$ is related to $x$ as

$$r = x b Z^{-1/3}; \quad b = \frac{\frac{3}{2} (\frac{1}{4} \pi)^{2/3}}{\frac{1}{4} (\frac{2}{3} b)^{2/3}} = 0.885 \quad (2)$$

(where we are using atomic units so $m_e e^2/\hbar^2 = 1$). The electric potential within an atom is given by

$$\phi(r) = \frac{Ze}{r} \chi \left( \frac{r Z^{1/3}}{b} \right) = \frac{Z^{4/3}}{b} \chi(x) \quad (3)$$

We point out that the Thomas-Fermi model does not apply for either very large or very small $x$; however, the major contribution to the scattering integral is from $x \approx 1$, and we would expect this model to give reasonably accurate results.

III. INTERACTION OF AN EDM WITH THE ATOMIC ELECTRIC FIELD

We are interested in calculating the spin-dependent neutron scattering length by the Born approximation for
either the $v \times E$ field or a neutron permanent electric dipole moment (EDM). Consider first the EDM interaction,

$$V(r) = -de\vec{r} \cdot \vec{E}(r)$$  \hspace{1cm} (4)

where $d$ is the dipole moment length, $e$ is the magnitude of the electron charge, $\sigma$ is a Pauli matrix, and $\vec{E}(r)$ is an electric field. The scattering amplitude (length) can be determined by use of the Born approximation,

$$a = -\frac{m_n}{2\pi\hbar^2} \int V(r)e^{i\vec{q} \cdot \vec{r}}d^3r$$  \hspace{1cm} (5)

Taking the momentum transfer $\vec{q}$ along $\hat{z}$ as the quantization axis, and using the fact that the electric field is spherically symmetric, we find

$$a = \sigma_z \frac{m_n}{2\hbar^2} \int_0^\infty E(r)e^{iqr\cos\theta} \cos\theta \sin\theta r^2drd\theta$$  \hspace{1cm} (6)

and the other components are zero because of symmetry. Taking $\vec{E}(r) = -\vec{d}(r)\hat{r}$, and using the Thomas-Fermi wavefunction, the scattering length can be written as, taking $\beta = bZ^{-1/3}$,

$$a = -\sigma_z \frac{m_n}{2\hbar^2} \beta Ze^2d \int_0^\infty [-\chi(x) + x\chi'(x)] e^{ix\beta q \cos\theta} \cos\theta \sin\theta dxdrd\theta$$  \hspace{1cm} (7)

which can be rewritten as

$$a = -\sigma_z \frac{m_n}{2\hbar^2} \beta dZe^2/3 f(\beta q)$$  \hspace{1cm} (8)

where $f(\beta q)$ is the imaginary part (the real part is zero) of the dimensionless integral in the previous equation. The Thomas-Fermi equation was numerically solved using a Runge-Kutta technique, and the integral numerically evaluated. The results, as a function of $\beta q$, are shown in Fig. 1.

For the case of Si, $Z = 14$, $\beta = 0.367$; a typical $q$ is approximately $2\pi/2\AA \times 0.5\AA$/a.u. giving $\beta q = 0.58$, and the dimensionless integral is about 1. Thus, the difference in the scattering length for the two spin states (along $\pm\vec{q}$) is

$$\Delta a = -2ibdZ^2/3 m_n/m_e = 2 \times 10^4d$$  \hspace{1cm} (9)

which leads to an spin rotation, on interference with the Si nuclear scattering amplitude ($a_0 = 4 \times 10^{-13}$ cm)

$$\Delta \phi = \frac{\Delta a}{a_0} = 4.7 \times 10^{16}d/cm$$  \hspace{1cm} (10)

implying that for $d = 5 \times 10^{-27}$ cm, a Bragg reflection from an Si crystal would give a rotation of $2 \times 10^{-10}$ rad.

\section*{IV. $\vec{v} \times \vec{E}$ Interaction}

Next, consider the $\vec{v} \times \vec{E}$ motional magnetic field interaction which couples to the neutron magnetic moment, which was first considered by Schwinger in 1948. The possibility of measuring effects from the motional field has been discussed in regard to non-centrosymmetric crystals (α-quartz) in which case a non-zero average electric field between scattering planes can exist. However, as has been pointed out, there is a $\vec{v} \times \vec{E}$ observable even for symmetric crystals.

The hamiltonian for the $\vec{v} \times \vec{E}$ interaction is

$$V(r) = -\vec{\mu} \cdot \left[\left(\frac{\vec{p}}{m_n c}\right) \times \vec{E}(r)\right]/2.$$  \hspace{1cm} (11)

For the Born approximation, we use the matrix element $\langle \vec{k}_2|V(r)|\vec{k}_1 \rangle = \vec{\mu} \cdot \frac{1}{2} (\vec{p}_{\vec{k}_2} - \vec{p}_{\vec{k}_1}) \times \vec{E}(r) - \vec{E}(r) \times \frac{\vec{p}_{\vec{k}_1} \cdot \vec{k}_1}{m_n c}$

$$\langle \vec{k}_2|\vec{p}|\vec{k}_1 \rangle = \hbar \langle \vec{k}_2|\vec{p}|\vec{k}_1 \rangle; \hspace{1cm} \langle \vec{k}_2|\vec{p}|\vec{k}_2 \rangle$$

which can be rewritten as

$$\langle \vec{k}_2|V(r)|\vec{k}_1 \rangle = -\vec{\mu} \cdot \frac{\hbar}{m_n c} \left(\vec{k}_1 + \vec{k}_2\right) \times \vec{E}(r)/2.$$  \hspace{1cm} (12)

Again, assume that $\vec{q}$ lies along $\hat{z}$; we note that $\vec{q} = \vec{k}_2 - \vec{k}_1$ is perpendicular to $\vec{k}_1 + \vec{k}_2$ because

$$(\vec{k}_2 - \vec{k}_1) \cdot (\vec{k}_1 + \vec{k}_2) = k_2^2 - k_1^2 = 0$$  \hspace{1cm} (13)

for elastic scattering. By symmetry, the effective electric field lies along $\hat{z}$, and if we assume $\vec{k}_1 + \vec{k}_2$ is along $\hat{y}$ and $\vec{q}$ (and has magnitude $2k \cos\theta_s$, $2\theta_s$ is the scattering angle), the Born approximation is

$$a = -\sigma_z \frac{m_n}{2\pi\hbar^2} \beta Z$$

$$\times \int E(\vec{r}) \cos\theta e^{iqr\cos\theta} \sin\theta d\theta d\varphi d\vec{r}$$  \hspace{1cm} (14)

which leads to a spin rotation, on interference with the Si nuclear scattering amplitude ($a_0 = 4 \times 10^{-13}$ cm)

$$\Delta a = -2ibdZ^2/3 m_n/m_e = 2 \times 10^4d$$  \hspace{1cm} (15)

where $\gamma$ is the neutron magnetic moment (-3 Hz/mG). Thus, the integral is identical to the EDM case, with a different multiplicative constant, and

$$\Delta a = -\frac{m_n}{2\pi\hbar^2} \frac{\hbar k \cos\theta_s \beta Z e}{c} \mu f(\beta q)$$  \hspace{1cm} (16)

or a spin rotation about $\hat{x}$ of

$$\Delta \phi \approx 4 \times 10^{-15} cm/4 \times 10^{-13} cm = 10^{-2} \text{ rad}$$  \hspace{1cm} (17)

per Bragg reflection from an Si crystal.
V. SEMI-CLASSICAL MODEL

If we assume there is no electron cloud around the nucleus, in Eq. (7) \( \chi = 1 \), and \( a_{edm} \propto 1/q \), which is equivalent to the high-momentum limit. We can estimate the EDM effect by taking a classical trajectory with impact parameter \( b \) relative to the nucleus. The time-integrated-electric-field-induced phase shift, assuming a spin in the the \( \hat{z} \) direction (propagation in \( \hat{x} \) direction) is given by

\[
\Delta \phi = -\int_{-\infty}^{\infty} \frac{edE}{hv} \, dx = -\frac{Ze^2}{h} \int_{-\infty}^{\infty} \frac{b}{[b^2+(x^2)^{1/2}]} \, dx
\]

which is essentially the same as before, in the high momentum limit, if we take \( b = a_{nuc} \).

VI. DISCUSSION

Comparing Eqs. (10) and (19), we see that the motional field spin rotation is on the order of \( 10^8 \) times larger than that due to an EDM with a magnitude that would be of interest in an improved experiment. Unfortunately, the effects cannot be switched on and off as in the case of the more conventional experiments based on spin precession in an applied electric field. Although the two scattering effects are proportional to \( \sigma_x \) and \( \sigma_z \) respectively, discrimination between the effects relies on an absolute determination of the polarization and scattering axes. One can also be concerned with the normal nuclear parity violation, which can combine with a misalignment to produce effects that mimic T-violation. This and other issues relevant for a realistic EDM scattering experiment are similar to those relating to a study of time reversal violating effects in slow neutron transmission through polarized matter for which the issues have been addressed in some detail; in particular, the constraints on near-perfect field and polarization alignment, and inability to discriminate effects due to misalignments, have been emphasized. The scattering angles constraints in a Bragg scattering EDM experiment are analogous to the constraints on the sample polarization axis in a neutron transmission experiment as discussed in [8]. Given the constraints (e.g., scattering angle and polarization alignment to \( 10^{-8} \) radian absolute accuracy which requires \( 10^{16} \) neutron counts to measure experimentally) achieving any significant increase in the limit for the neutron EDM would seem a daunting task.

[1] C.G. Shull and R. Nathans, Phys. Rev. Lett. 19, 384 (1967).