INELASTIC MAGNETIC ne SCATTERING AT SMALL ANGLES

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Inelastic magnetic scattering of neutrons by electrons is considered. It is shown that at small angles and small momentum transfers deviations from the usual behavior of the scattered wave appear. As a consequence of this, the relation between the differential scattering cross section and the magnetic susceptibility tensor of matter changes appreciably.

As is well known,[1] the theory of magnetic ne-scattering developed in articles[2,3] leads to ambiguous results for the description of the scattering at zero angle. In article[4] it was shown that in the case of elastic scattering the results obtained in[2,3] are valid only upon fulfillment of the condition $\theta \gg 1/\sqrt{kr}$ (θ is the scattering angle). If this condition is violated, then the usual asymptotic behavior $f(\theta)r^{-1}e^{ikr}$ for the scattered wave is incorrect because additional terms proportional to $(e^{i\mathbf{g}\cdot\mathbf{r}} - 1)/i\mathbf{g}\cdot\mathbf{r}$ ($\hbar\mathbf{g}$ is the momentum transfer) appear in the scattering amplitude; as is evident, these terms are important only at small angles $\mathbf{g}\cdot\mathbf{r} \lesssim 1$. It is natural that in the limit of small angles and small momentum transfer anomalies should also appear in the amplitude describing inelastic scattering. To be sure from an analysis of the condition $\mathbf{g}\cdot\mathbf{r} \lesssim 1$ in the case of inelastic scattering it might follow that the contribution of the additional terms to the scattering amplitude, even at zero angle, would be appreciable only at very small momentum transfers $|g|r \lesssim 1$, i.e., for $r \sim 1$ cm, $|g| \lesssim 1\ \text{cm}^{-1}$. However, such a conclusion is not correct. As will be shown below, in the general case of inelastic scattering two conditions exist, whose fulfillment leads to the appearance of anomalies in the asymptotic behavior of the wave function. One of these restricts the scattering angle and agrees with the analogous condition in the case of elastic scattering, i.e., $\theta \lesssim 1/\sqrt{kr}$. The second condition is imposed on the momentum transfer and, as will be shown below, has the form $(k_b - k)^2 r/2k \lesssim 1$.

In fact, in this case the wave function is determined by the expression

$$\Psi_{sc} = -\frac{m}{\hbar^2\pi^2}\sum_b |b\rangle\langle b|\sum_{i=1}^N \exp(i\mathbf{k}\boldsymbol{\xi}_i)\int d^3p\,\frac{\exp(i\mathbf{p}(\mathbf{r}-\boldsymbol{\xi}_i))}{p^2 - k_b^2 - i\varepsilon}\times\left[\frac{(\boldsymbol{\mu}_n(\mathbf{k}-\mathbf{p}))(\boldsymbol{\mu}_i(\mathbf{k}-\mathbf{p}))}{(\mathbf{k}-\mathbf{p})^2} - \boldsymbol{\mu}_n\boldsymbol{\mu}_i\right]|a\rangle, \tag{1}$$

where μ_n and μ_i are, respectively, the magnetic moment operators of the neutron and of the i-th electron; k is the wave vector of the incident neutrons; m is the neutron mass; $|a\rangle$ and $|b\rangle$ are the wave functions of the scatterer before and after the collision; ξ denotes the coordinates of the electrons; $k_b^2 = k^2 + 2m\hbar^{-2}(E_a - E_b)$; E_a and E_b denote the internal energies of the scattering system in states a and b.

Having used the well-known identity

$$\frac{1}{AB} = \int_0^1 dz\,\frac{1}{[Az + B(1-z)]^2} \tag{2}$$

we integrate Eq. (1) over the momentum **p**. As a result we obtain

$$\Psi_{sc} = -\frac{2m}{\hbar^2}\sum_b |b\rangle\langle b|\sum_{i=1}^N \exp(i\mathbf{k}\boldsymbol{\xi}_i)\times\Big[-\boldsymbol{\mu}_n\boldsymbol{\mu}_i\frac{\exp(ik_b|\mathbf{r}-\boldsymbol{\xi}_i|)}{|\mathbf{r}-\boldsymbol{\xi}_i|} - \frac{i}{2}\exp(i\mathbf{k}(\mathbf{r}-\boldsymbol{\xi}_i))\times(\boldsymbol{\mu}_n\nabla_r)(\boldsymbol{\mu}_i\nabla_r)\int_0^1 dz\,\frac{1}{\sqrt{k^2z^2+\varkappa^2 z}}\exp(-i\mathbf{k}(\mathbf{r}-\boldsymbol{\xi}_i)z)\times\exp(i\sqrt{k^2z^2+\varkappa^2 z}\,|\mathbf{r}-\boldsymbol{\xi}_i|)\Big]|a\rangle\quad\left(\varkappa^2 = \frac{2m}{\hbar^2}(E_a - E_b)\right). \tag{3}$$

Let us introduce the new variable

$$z = \frac{\varkappa^2}{4k^2}\left(t + \frac{1}{t}\right) - \frac{\varkappa^2}{2k^2}.$$

Integrating with respect to the parameter t, taking account of the fact that $\mathbf{k}\cdot(\mathbf{r} - \boldsymbol{\xi}_i) \approx k|\mathbf{r} - \boldsymbol{\xi}_i|$, if we analyze ψ_{sc} in the angular range $\theta \ll 1/\sqrt{kr}$ of interest to us we finally obtain

$$\Psi_{sc} = -\frac{2m}{\hbar^2}\sum_b |b\rangle\langle b|\sum_{i=1}^N \exp(i\mathbf{k}\boldsymbol{\xi}_i)\times[(\boldsymbol{\mu}_n\mathbf{e})(\boldsymbol{\mu}_i\mathbf{e}) - (\boldsymbol{\mu}_n\boldsymbol{\mu}_i)]\frac{\exp(ik_b|\mathbf{r}-\boldsymbol{\xi}_i|)}{|\mathbf{r}-\boldsymbol{\xi}_i|}|a\rangle - \frac{2m}{\hbar^2}\sum_b |b\rangle\langle b|\sum_{i=1}^N \exp(i\mathbf{k}\boldsymbol{\xi}_i)[\boldsymbol{\mu}_n\boldsymbol{\mu}_i - 3(\boldsymbol{\mu}_n\mathbf{e})(\boldsymbol{\mu}_i\mathbf{e})]\times g(k, k_b, |\mathbf{r}-\boldsymbol{\xi}_i|)\frac{\exp(ik_b|\mathbf{r}-\boldsymbol{\xi}_i|)}{|\mathbf{r}-\boldsymbol{\xi}_i|}|a\rangle,$$

$$g(k, k_b, R) = \frac{(k_b - k)(k_b + k)}{8k^2}\left[\frac{k_b + k}{k_b - k} - \exp(i(k - k_b)R)\right] + \frac{i}{4kR}[1 - \exp(i(k - k_b)R)] + i\frac{(k_b - k)^2(k_b + k)^2}{16k^3}R\times\exp\left(i\frac{(k_b - k)^2}{2k}R\right)\left[\mathrm{Ei}\left(-i\frac{(k_b - k)^2}{2k}R\right) - \mathrm{Ei}\left(-i\frac{(k_b - k)(k_b + k)}{2k}R\right)\right], \tag{4}$$

$\mathbf{e} = \mathbf{r}/r$, Ei(x) is the exponential integral. The first term in (4) corresponds to the usual expression for a scattered wave (see, for example,[5]).

Let us consider the second term in more detail. If the condition $z_1 \equiv (k_b - k)^2 R/2k \gg 1$ is fulfilled (in this case $z_2 \equiv (k_b - k)(k_b + k)R/2k = z_1(k_b + k)/k_b - k)$ is also much larger than unity), the function $g(k, k_b, R) \ll 1$ and the second term may be neglected. However, if the value of z_1 becomes comparable with unity or smaller (for thermal neutrons with $R \sim 1$ cm, this corresponds to a momentum transfer of the order of $10^4\ \text{cm}^{-1}$ or $E_a - E_b \sim 10^{-6}$ eV), then the function

$g(k, k_b, R) \sim 1$ and it is impossible to neglect the second term. Here we note that under the indicated conditions, one can discard the term containing the function $\mathrm{Ei}(-i(k_b - k)(k_b + k)R/2k)$ in the expression for the quantity $g(k, k_b, R)$ because for $R > 1/k$ it is much smaller than unity.

Thus, for simultaneous fulfillment of the conditions

$$\frac{(k_b-k)^2}{2k}R \leqslant 1, \qquad \frac{(k_b-k)(k_b+k)}{2k}R \gtrsim 1$$

(for thermal neutrons with $R \sim 1$ cm this corresponds to

$$1\,\mathrm{cm}^{-1} \leqslant |k_b - k| \lesssim 10^4\,\mathrm{cm}^{-1} \text{ or } 10^{-10}\,\mathrm{eV} \lesssim |E_a - E_b| \lesssim 10^{-6}\,\mathrm{eV})$$

the wave function describing elastic scattering is determined by the following expression:

$$\Psi_{sc} = -\frac{2m}{\hbar^2}\sum_{\alpha=1}^{3}\{(\mu_n e)e^\alpha - \mu_n^\alpha + [\mu_n^\alpha - 3(\mu_n e)e^\alpha]g_0(k, k_b, r)\}$$
$$\times \frac{\exp(ik_b r)}{r}\sum_{b\neq a}|b\rangle\langle b|\sum_{i=1}^{N}\exp\left(i\left(\mathbf{k} - k_b\frac{\mathbf{r}}{r}\right)\xi_i\right)\mu_i^\alpha|a\rangle,$$
$$g_0(k, k_b, r) = \frac{(k_b+k)^2}{8k^2} + \frac{i}{4kr} + i\frac{(k_b-k)^2(k_b+k)^2}{16k^3}r$$
$$\times \exp\left(i\frac{(k_b-k)^2}{2k}r\right)\mathrm{Ei}\left(-i\frac{(k_b-k)^2}{2k}r\right). \qquad (5)$$

Finally, if z_2 becomes smaller than unity (in this case z_1 is also smaller than unity), then in the function $g(k, k_b, r)$ it is necessary to take all terms into account. In connection with the transition to elastic scattering $k_b \to k$, $g(k, k_b, r) \to 1/2$ the scattered wave (4) goes over into the previously obtained expression for the wave function describing elastic ne-scattering.[4]

Thus, from an analysis of expression (4) it follows that deviations from the usual behavior of the scattered wave appear in elastic scattering in the region of small angles $\theta \ll 1/\sqrt{kr}$ upon fulfillment of the condition $(k_b - k)^2 r/2k \lesssim 1$. It is clear that under the conditions indicated above the expression for the differential cross section will also change substantially. Thus, the cross section for inelastic scattering of unpolarized neutrons with

$$\frac{(k_b-k)^2}{2k}r \leqslant 1, \qquad \frac{(k_b-k)(k_b+k)}{2k}r \gtrsim 1$$

has the form (compare, for example, with[5])

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{inel}} = \left(\frac{2m}{\hbar^2}\mu_n\right)^2 \sum_a \rho_a \sum_{b\neq a}\frac{k_b}{k}$$
$$\times \sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\{\delta_{\alpha\beta}[1 - g_0(k, k_b, r) - g_0^+(k, k_b, r) + g_0^+(k, k_b, r)g_0(k, k_b, r)]$$
$$+ e_\alpha e_\beta[-1 + g_0(k, k_b, r) + g_0^+(k, k_b, r) + 3g_0(k, k_b, r)g_0^+(k, k_b, r)]\}\langle a|\sum_{i=1}^{N}$$
$$\times \exp\left(-i\left(\mathbf{k} - k_b\frac{\mathbf{r}}{r}\right)\xi_i\right)\mu_i^\alpha|b\rangle\langle b|\sum_{j=1}^{N}\exp\left(i\left(\mathbf{k} - k_b\frac{\mathbf{r}}{r}\right)\xi_j\right)\mu_j^\beta|a\rangle. \qquad (6)$$

It is well known that the differential scattering cross section can be directly expressed in terms of the magnetic susceptibility tensor of matter (see, for example,[5]). Naturally the relation between the magnetic susceptibility tensor and the cross section is also changed in the case under consideration. It is necessary, of course, to take the indicated property into account in connection with a discussion of the behavior of the differential cross section in the limit of very small angles and small momentum transfer ($\mathbf{k} - k_b\mathbf{r} \to 0$) (see, for example,[6]). Here we note that the differential cross section integrated over a range of angles larger than the critical angle agrees with the cross section obtained by using the usual expression for the scattering amplitude, also integrated over the indicated range of angles. In conclusion we note that the identity (2) enables us to obtain an explicit expression for the wave function describing elastic magnetic scattering in an arbitrary coordinate system (in article[4] the wave function was obtained in the case when the z axis was directed along the vector $\mathbf{k}$), which has the form

$$\Psi_{sc} = -\frac{2m}{\hbar^2}\left[\frac{(\mu_n\mathbf{g})(\mu\mathbf{g})}{g^2} - \mu_n\mu\right]\frac{\exp(ikr)}{r}$$
$$-\frac{2m}{\hbar^2}\left[\frac{1}{2}\mu_n\mu - \frac{1}{2}\frac{(\mu_n\mathbf{r})(\mu\mathbf{r})}{r^2} - \frac{(\mu_n\mathbf{g})(\mu\mathbf{g})}{g^2}\right]$$
$$\times\frac{\exp(i\mathbf{g}\mathbf{r}) - 1}{i\mathbf{g}\mathbf{r}}\frac{\exp(ikr)}{r}, \qquad (7)$$

where $\mathbf{g} = \mathbf{k} - (k\mathbf{r}/r)$ is the momentum transfer.

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