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Electron Scattering with Spin-Orbit Interaction and the Mott Theorem

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Abstract From an unpolarized electron beam the general self-adjoint interactian Hamiltonian composed of an orbital part plus a spin orbit part gives a final polarization equal to zero when the calculations are performed in the Born approximation. This theorem, proved by Mott for the case of a spherically symmetric target, is shown to have more general validity.

In 1929 Mott[1] showed that a Hamiltonian of spherical symmetry composed of a spin independent potential plus a spin-orbit coupling term does not lead to polarization effects when the calculations are performed in Born approximation. In spite of this, Fermi[2], studying proton scattering by nucleons in the Born approximation, obtained a final polarization different from zero. The contradiction between Mott and Fermi is only apparent. In both cases the scattering potentials are spherically symmetric but there is an essential difference between them. In Mott paper the scattering potential is Hermitian, while Fermi assumed a scattering potential of the form

$$H = (1+i\xi)\ \varepsilon V(r) + \left[-\eta\,\frac{1}{r}\ \frac{dV(r)}{dr}\ (\vec{L}.\vec{\sigma})\right] \qquad (1)$$

where $V(r)$ is the spherically symmetric potential.

$\eta = -\varepsilon\hbar/4\mu^2c^2$, where ε is the electronic charge, $\vec{L}$ the electron angular momentum, $\vec{\sigma}$ the Pauli spin operator, μ is the electron mass, c is the speed of light in vacuum and ξ is a constant describing absorption.

The first term in eq. (1) has both real and imaginary parts. In this way, an artificial interference between the orbital and the spin orbit part is obtained, which results in a final polarization which

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is different from zero. However, eq. (1) violates the very important Hermitian property of Hamiltonian operators and consequently the quantum-mechanical conservation of probability. Fermi's intention was, of course, to describe an absorbing system with such Hamiltonian. The polarization effects, however, which are thereby introduced, are an artefact.

In order to demonstrate that the Mott theorem is valid for any geometry, we assume an interaction Hamiltonian of the form

$$H = \varepsilon V(\vec{r}) + \eta(-\vec{\nabla}_{\vec{r}} V(\vec{r}) \wedge \vec{p}) \cdot \vec{\sigma} \tag{2}$$

where $\vec{p} = -i\hbar\vec{\nabla}_{\vec{r}}$ and $V(\vec{r})$ is a general Hermitian potential not necessarily spherically symmetric. This point gives precisely the generalization of the Mott theorem.

The operator in eq. (2) is in spin-space a (2×2) matrix of the form

$$H = a1 + \vec{b}.\vec{\sigma} = \begin{pmatrix} a + b_z & b_x - ib_y \\ b_x + ib_y & a - b_z \end{pmatrix} \tag{3}$$

The scattering matrix in spin-space has the form

$$M = A1 + \vec{B}.\vec{\sigma} \tag{4}$$

In Born approximation it is

$$M = -\frac{\mu}{2\pi\hbar^2}\{\langle\vec{k}'|\varepsilon V(\vec{r})|\vec{k}\rangle 1 + \eta\langle\vec{k}'|-\vec{\nabla}_{\vec{r}} V(\vec{r}) \wedge \vec{p}|\vec{k}\rangle \cdot \vec{\sigma}\} \tag{5}$$

The kets

$$|\vec{k}\rangle = e^{i\vec{k}.\vec{r}} \quad \text{and} \quad |\vec{k}'\rangle = e^{i\vec{k}'.\vec{r}} \tag{6}$$

denote, respectively, the incoming and outgoing wave of an electron of the beam.

The direct comparison between (4) and (5) leads to

$$A = -\frac{\mu}{2\pi\hbar^2}\langle\vec{k}'|\varepsilon V(\vec{r})|\vec{k}\rangle = -\frac{\mu\varepsilon}{2\pi\hbar^2} V_{\vec{K}} \tag{7}$$

and

$$\vec{B} = -\frac{\mu\eta}{2\pi\hbar^2} \langle \vec{k}' | -\vec{\nabla}_{\vec{r}} V(\vec{r}) \wedge \vec{p} \, | \vec{k} \rangle \tag{8}$$

where

$$V_{\vec{K}} = \int d^3r \, e^{i\vec{K}.\vec{r}} \, V(\vec{r}) \tag{9}$$

and

$$\vec{K} = \vec{k} - \vec{k}' \tag{10}$$

The development of eq. (8) leads to

$$\vec{B} = \frac{\mu\eta}{2\pi\hbar} \left[\int d^3r \, e^{i\vec{K}.\vec{r}} \, \vec{\nabla}_{\vec{r}} \, V(\vec{r}) \right] \wedge \vec{k} \tag{11}$$

In this iritegration we have

$$\vec{\nabla} = i\vec{K} = i(\vec{k} - \vec{k}') \tag{12}$$

so that

$$\vec{B} = \frac{\mu\eta}{2\pi\hbar} \, i \, V_{\vec{K}} \, \vec{\nu} \tag{13}$$

where

$$\vec{\nu} = \vec{k} \wedge \vec{k}' \tag{14}$$

The quantity 2 Re $(A\vec{B}^*)$ becomes

$$2 \, \mathrm{Re}(A\vec{B}^*) = \frac{\mu^2\varepsilon\eta}{4\pi^2\hbar^3} \{ -i |V_{\vec{K}}|^2 \, \vec{\nu} + i |V_{\vec{K}}|^2 \, \vec{\nu} \} = 0$$

The quantity $\vec{B} \wedge \vec{B}^*$ is equal to zero because B and B^* are proportional to $\vec{\nu}$.

We obtained for the polarization $\vec{P}$, the asymmetry $\vec{A}$ and the difference $\vec{P} - \vec{A}$ the results

$$\vec{P} = \frac{\mathrm{tr}(MM^+\vec{\sigma})}{\mathrm{tr}(MM^+)} = \frac{2\mathrm{Re}(A\vec{B}^*) + i(\vec{B} \wedge \vec{B}^*)}{\Delta} = 0$$

$$\vec{A} = \frac{\mathrm{tr}(M^+M\vec{\sigma})}{\mathrm{tr}(MM^+)} = \frac{2\mathrm{Re}(A\vec{B}^*) - i(\vec{B} \wedge \vec{B}^*)}{\Delta} = 0$$

$$\vec{P} - \vec{A} = \frac{\mathrm{tr}\{[M, M^+]\vec{\sigma}\}}{\mathrm{tr}(MM^+)} = \frac{2i(\vec{B} \wedge \vec{B}^*)}{\Delta} = 0$$

where

$$\Delta = |A|^2 + |B|^2 \neq 0$$

The polarization effects are zero in the Born approximation and the theorem is thus proved.

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REFERENCES

1. N.F.Mott, Proc. Roc. Soc., p. 425 (1929).
2. E.Fermi, Nuovo Cimento *10*, 407 (1954).

Resumo

A partir de um feixe eletrônico não polarizado, o Hamiltoniano auto-adjunto geral, composto de uma parte orbital e de outra de interação de spin-orbita leva a uma polarização final igual a zero, quando os cãlculos são realizados no contexto da aproximação de Born. Este teorema foi mostrado por Mott para caso de alvos esfericamente simétricos. O teorema é válido para qualquer geometria,. não necessarlamente esférica, e nesta nota, procedemos a sua generalização.