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Ruderman-Kittel-Kasuya-Yosida polarization across a potential well in one dimension

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Abstract

The RKKY spin polarization due to a point field is calculated for an electron gas with a reflectionless potential well. An approximation which uses a space dependent Fermi wave number is introduced. It follows remarkably well the exact result. For a class of potentials it is shown that the integrated spin polarisation equals the Pauli susceptibility multiplied by the coupling constant and the mean probability density of the electron states of the Fermi surface at the position of the point field.

Key-words: Spin-spin couplings; Magnetic films; Magnetic-multilayers.

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I. INTRODUCTION

Experiments with layered ferromagnetic structures raised the problem of the spin polarization of the conduction electrons in metals in inhomogeneous situations. Some results exist for finite metals [1] [2]. An important question is how the spin polarization crosses a region with a different metal. This problem was repeatedly adressed [3]– [8]. The present work discusses a one-dimensional model with a particular localized potential which lends itself to analytic treatment.

II. THE MODEL

Consider a non-interacting electron gas in unlimited one-dimensional space. The electrons are subject to a localized potential of width λ

$$V(x) = -V_0 \,\mathrm{sech}^2(\lambda x) \tag{1}$$

$$V_0 = 2\lambda^2 \hbar^2/(2m), \tag{2}$$

where m is the mass of an electron. With Eq. (2) the potential has the remarkable property of being reflectionless [9]. It has been chosen for the simplicity of the wave-functions and the spectrum. This consists of a continuous part

$$\phi_{k,s}(x) = \frac{-ik + \lambda\,\tanh(\lambda x)}{\sqrt{k^2+\lambda^2}}\;\mathrm{e}^{ikx}\,|s\rangle, \qquad E_k = \frac{\hbar^2 k^2}{2m}, \tag{3}$$

and one bound state

$$\phi_{b,s}(x) = \sqrt{\frac{\lambda}{2}}\;\mathrm{sech}(\lambda x)\,|s\rangle, \qquad E_b = -\frac{\hbar^2\lambda^2}{2m}. \tag{4}$$

$s = \pm\frac{1}{2}$ is the spin variable. The states with $|k| \le k_F$ are filled, where $k_F = \pi n$ is determined by the asymptotic particle density n of the electrons.

The perturbing Hamiltonian, which represents a point field at position a that acts on the spins of the electrons with strength γ, is

$$H' = -\gamma\,\delta(x-a)\,\frac{\sigma_z}{2}, \tag{5}$$

where σ_z is the Pauli matrix for the z direction. The spin polarization linear in γ can be obtained from the first order perturbation of the wave functions alone without any change of occupation, provided the singularities are handled with principle part integrations [10]. With Eq. (5) the matrix elements are immediate, and the perturbed wave functions become

$$\psi_{k,s}(x) = \phi_{k,s}(x) - \gamma\, s\, \frac{2m}{\hbar^2}\,\frac{1}{2\pi}\int_{-\infty}^{\infty} dk'\, \frac{\phi^*_{k',s}(a)\,\phi_{k,s}(a)}{k^2-k'^2}\phi_{k',s}(x) - \gamma\, s\,\frac{2m}{\hbar^2}\,\frac{\phi^*_{b,s}(a)\,\phi_{k,s}(a)}{k^2+\lambda^2}\,\phi_{b,s}(x) \tag{6}$$

$$\psi_{b,s}(x) = \phi_{b,s}(x) + \gamma\, s\, \frac{2m}{\hbar^2}\,\frac{1}{2\pi}\int_{-\infty}^{\infty} dk'\, \frac{\phi^*_{k',s}(a)\,\phi_{b,s}(a)}{\lambda^2+k'^2}\phi_{k',s}(x). \tag{7}$$

The spin polarization is given by the terms linear in γ of

$$P(x,a) = \sum_s \int_{-k_F}^{k_F} dk\, \psi^*_{k,s}(x)\,\frac{\sigma_z}{2}\,\psi_{k,s}(x) + \sum_s \psi^*_{b,s}(x)\,\frac{\sigma_z}{2}\,\psi_{b,s}(x). \tag{8}$$

In combination with Eq. (6) two integrations have to be performed. Yafet [3] has made it clear that the singularity $k = k' = 0$ requires special care in the one-dimensional case. The result depends on the order of the integrations. The physically meaningful result is obtained when the integration over k is done first. Since all expressions are diagonal in the spin variables, these will be suppressed; the factors $\frac{1}{2}$ in Eq. (9) stand for $\sum_s s^2$.

$$\begin{aligned} P(x,a) = & -\frac{2m}{\hbar^2}\,\gamma\,\frac{1}{2}\int_{-\infty}^{\infty}\frac{dk'}{2\pi}\int_{-k_F}^{k_F}\frac{dk}{2\pi}\,\frac{\phi^*_k(x)\,\phi^*_{k'}(a)\,\phi_k(a)\,\phi_{k'}(x)}{k^2-k'^2} \;+\; \text{c.c.} \\ & -\frac{2m}{\hbar^2}\,\gamma\,\frac{1}{2}\int_{-k_F}^{k_F}\frac{dk}{2\pi}\,\frac{\phi^*_k(x)\,\phi^*_b(a)\,\phi_k(a)\,\phi_b(x)}{k^2+\lambda^2} \;+\; \text{c.c.} \\ & +\frac{2m}{\hbar^2}\,\gamma\,\frac{1}{2}\int_{-\infty}^{\infty}\frac{dk'}{2\pi}\,\frac{\phi^*_b(x)\,\phi^*_{k'}(a)\,\phi_b(a)\,\phi_{k'}(x)}{\lambda^2+k'^2} \;+\; \text{c.c.}\,. \end{aligned} \tag{9}$$

Defining

$$C_k = \frac{(k^2+\lambda^2 T)\,\cos(kz) - k\lambda S\,\sin(kz)}{k^2+\lambda^2} \tag{10}$$

$$T = \tanh(\lambda x)\,\tanh(\lambda a) \tag{11}$$

$$S = |\tanh(\lambda x) - \tanh(\lambda a)| \tag{12}$$

$$z = |x-a|, \tag{13}$$

Eq. (9) becomes

$$P(x,a) = -\frac{2m}{\hbar^2}\,\frac{\gamma}{4\pi}\left\{I_1 + I_2 + I_3\right\} \tag{14}$$

$$I_1 = \frac{2}{\pi}\left[\int_0^\infty dk' \int_0^\epsilon dk \;-\; \int_0^\epsilon dk \int_0^\infty dk'\right] \frac{C_k C_{k'}}{k^2 - k'^2} \tag{15}$$

$$I_2 = \int_0^{k_F} \frac{dk}{k}\,\frac{1}{(k^2+\lambda^2)^2}\left\{ \left[\left(k^2+\lambda^2 T\right)^2 - (k\lambda S)^2\right]\,\sin(2kz) + 2\lambda S k\,\left(k^2+\lambda^2 T\right)\,\cos(2kz)\right\} \tag{16}$$

$$\begin{aligned} I_3 = 2\lambda\left[\mathrm{e}^{-\lambda z}(T-1-S) + \,\mathrm{sech}(\lambda x)\,\mathrm{sech}(\lambda a)\right] \int_0^{k_F} dk\,\frac{C_k}{(k^2+\lambda^2)} \\ -\frac{\pi}{2}\,\mathrm{sech}(\lambda x)\,\mathrm{sech}(\lambda a)\,\mathrm{e}^{-\lambda z}\left[T + 1 + \lambda z(T-1-S)\right]. \end{aligned} \tag{17}$$

The two integrations of I_1 commute everywhere exept in the neighbourhood of the singularity $k = k' = 0$, so that the integration over k' can be taken from zero to an infinitesimal η. C_k is regular at the singularity and takes the value T. Then [3]

$$I_1 = \frac{T^2}{\pi}\left\{ f\left(\frac{-\eta}{\epsilon}\right) - f\left(\frac{\eta}{\epsilon}\right) + f\left(\frac{-\epsilon}{\eta}\right) - f\left(\frac{\epsilon}{\eta}\right)\right\} = -\frac{\pi}{2}\,T^2, \tag{18}$$

where $f(x) = -\int_0^x dy\,\ln(|1-y|)/y$ is the Dilogarithm function [12]. As a limiting case let both x and a be on the same side of the potential and far away from it, i.e.

$$x, a \gg \lambda \qquad \text{or} \qquad -x, -a \gg \lambda. \tag{19}$$

In this case $T = 1$ and $S = 0$. Thus

$$P(x,a) = \frac{2m}{\hbar^2}\,\frac{\gamma}{4\pi}\,\left\{\frac{\pi}{2} - \mathrm{Si}(2k_F z)\right\}, \tag{20}$$

which is the RKKY result for a one dimensional homogeneous space [11] [3]. Note that the terms that were neglected were exponentionally small, in agreement with the reflection free property of the potential. Eq. (14) is plotted in Figs. 1–3 for different situations. In general $P(a,a) = \frac{2m}{\hbar^2}\,\frac{\gamma}{4\pi}$ independent of a and λ.

III. INTEGRATED POLARIZATION

We consider now the influence of the potential on the integrated polarisation. This can be done starting again with Eq. (9) and inverting the sequence of integrations

$$\mathcal{P}(a) = \int_{-\infty}^{\infty} P(x,a)\,dx \tag{21}$$

$$= \frac{\gamma}{2}\,\frac{2m}{\hbar^2}\int_{-\infty}^{\infty}\frac{dk'}{2\pi}\int_{-k_F}^{k_F}\frac{dk}{2\pi}\int_{-\infty}^{\infty}dx\,\frac{\phi_k^*(x)\,\phi_{k'}^*(a)\,\phi_k(a)\,\phi_{k'}(x)}{k'^2-k^2} \;+\; \text{c.c.}\,. \tag{22}$$

The remaining terms in Eq. (9) do not contribute because of the ortogonality between ϕ_k and ϕ_b. With

$$\int_{-\infty}^{\infty} dx\,\phi_k^*(x)\,\phi_{k'}(x) = 2\pi\,\delta(k-k') \tag{23}$$

and the change of variables $k' = k + q$ this becomes

$$\mathcal{P}(a) = \frac{\gamma}{4\pi}\,\frac{2m}{\hbar^2}\int_{-\infty}^{\infty}dq\,\frac{\delta(q)}{q}\int_{-k_F}^{k_F}\frac{dk}{2k+q}\left[\phi_{k+q}^*(a)\,\phi_k(a)+\phi_{k+q}(a)\,\phi_k^*(a)\right]. \tag{24}$$

In view of the factor $\delta(q)$ it is sufficient to retain up to linear terms in q, so that the bracket can be replaced by

$$2\,|\phi_k(a)|^2 + \left[\frac{d\phi_k^*}{dk}\phi_k + \frac{d\phi_k}{dk}\phi_k^*\right] q = 2\,|\phi_k(a)|^2 + \frac{d}{dk}\,|\phi_k(a)|^2\;q. \tag{25}$$

Thus

$$\mathcal{P}(a) = \frac{\gamma}{4\pi}\,\frac{2m}{\hbar^2}\,(K_1+K_2), \tag{26}$$

where

$$K_1 = \int_{-\infty}^{\infty}dq\,\frac{\delta(q)}{q}\int_{-k_F}^{k_F}dk\,\frac{2\,|\phi_k(a)|^2}{2k+q} \tag{27}$$

$$K_2 = \int_{-k_F}^{k_F}\frac{dk}{2k}\,\frac{d}{dk}\,|\phi_k(a)|^2. \tag{28}$$

Here

$$|\phi_k(a)|^2 = \frac{k^2+\lambda^2 U}{k^2+\lambda^2}, \qquad U = \tanh^2(\lambda a), \qquad \frac{d}{dk}\,|\phi_k|^2 = 2k\frac{\lambda^2(1-U)}{(k^2+\lambda^2)^2}. \tag{29}$$

Then

$$K_1 = \int_{-\infty}^{\infty} dq\, \frac{\delta(q)}{q} \int_{-k_F}^{k_F} dk\, 2\, |\phi_k(a)|^2\, \frac{1}{2k+q} \tag{30}$$

$$= \int_{-\infty}^{\infty} dq\, \frac{\delta(q)}{q} \left\{ -\left(1 + \frac{4\lambda^2(U-1)}{4\lambda^2+q^2}\right) \ln\left|\frac{q+2k_F}{q-2k_F}\right| + \frac{4\lambda(U-1)q}{4\lambda^2+q^2} \arctan\left(\frac{k_f}{\lambda}\right)\right\} \tag{31}$$

$$= \int_{-\infty}^{\infty} dq\, \delta(q) \left\{ \frac{U}{k_F} + \frac{U-1}{\lambda} + O(q^2)\right\} \tag{32}$$

$$= \frac{U}{k_F} + \frac{U-1}{\lambda} \arctan\left(\frac{k_F}{\lambda}\right). \tag{33}$$

The second integral K_2 becomes:

$$K_2 = \lambda^2(U-1) \int_{-k_F}^{k_F} \frac{dk}{(k^2+\lambda^2)^2} \tag{34}$$

$$= (1-U)\left\{ \frac{k_F}{k_F^2+\lambda^2} + \frac{1}{\lambda} \arctan\left(\frac{k_F}{\lambda}\right)\right\}. \tag{35}$$

Combining the two terms gives

$$\mathcal{P}(a) = \frac{\gamma}{4\pi}\, \frac{2m}{\hbar^2}\, \frac{|\phi_{k_F}(a)|^2}{k_F} \tag{36}$$

$$= \frac{\gamma}{4\pi}\, \frac{2m}{\hbar^2}\, \frac{1}{k_F} \left[1 - \frac{\lambda^2}{k_F^2+\lambda^2}\, \mathrm{sech}^2(\lambda a)\right]. \tag{37}$$

Eq. (36) shows that the integrated polarization $\mathcal{P}(a)$ is proportional to the probability density of an electron in the Fermi level to be at a. With the reflectionless potential the situation can arise that while a is outside the range of the potential, this overlaps with the polarization. It is remarkable that in this situation the integrated polarization $\mathcal{P}(a)$ is unchanged. In the Appendix we show that the result Eq. (36) can be generalized to a large class of potentials and to three dimensions.

An integral over $\mathcal{P}(a)$ is the integrated spin polarization due to a homogeneous field γ. Of course, this diverges for an infinite sample. However, the integral over the difference between $\mathcal{P}(a)$ and its asymptotic value is finite and has the value

$$\int_{-\infty}^{\infty} da\, \left[\mathcal{P}(a) - \frac{\gamma}{4\pi}\, \frac{2m}{\hbar^2}\, \frac{1}{k_F}\right] = -\frac{\gamma}{4\pi}\, \frac{2m}{\hbar^2}\, \frac{1}{k_F}\, \frac{2\lambda}{k_F^2+\lambda^2}. \tag{38}$$

This is the change of the integrated Pauli spin polarization induced by the potential.

IV. AN APPROXIMATION WITH A SPACE DEPENDENT FERMI VECTOR

Since in this case the exact spin polarization is known, it is tempting to compare it with an approximation, which uses Eq. (20), however, with a local Fermi wave number. The quantity $2k_F|x-a|$ in Eq. (20) is replaced by

$$X = \left| 2\int_a^x dx'\, k_F(x') \right| . \tag{39}$$

In one dimension $k_F(x) = \pi n(x)$, where $n(x)$ is the particle density.

From Eq. (3) and (4)

$$\begin{aligned} n(x) &= \int_{-k_F}^{k_F} \frac{dk}{2\pi}\, \frac{k^2+\lambda^2\tanh^2(\lambda x)}{k^2+\lambda^2} + \frac{\lambda}{2}\,\mathrm{sech}^2(\lambda x) && (40)\\ &= \frac{k_F}{\pi} + \frac{\lambda}{2}\,\mathrm{sech}^2(\lambda x)\left[1-\frac{2}{\pi}\arctan\left(\frac{k_F}{\lambda}\right)\right], && (41) \end{aligned}$$

where k_F is the asympthotic Fermi wave number.

$$X = 2k_F \left| x' + \frac{\pi}{2}\frac{1}{k_F}\tanh(\lambda x')\left[1-\frac{2}{\pi}\arctan\left(\frac{k_F}{\lambda}\right)\right]\right| \;\Bigg|_{x'=a}^{x} . \tag{42}$$

The second term produces a phase shift δ. In the limit $a=-\infty,\ x=\infty$ it amounts to

$$\delta = 2\pi\left[1-\frac{2}{\pi}\arctan\left(\frac{k_F}{\lambda}\right)\right]. \tag{43}$$

Thus if $k_F=\lambda$ then $\delta=\pi$. The phase shifts becomes evident in Fig. 3.

V. CONCLUSIONS

The problem of the spin susceptibility in general inhomogeneous situations is complex even in one dimension. However, in two cases the problem was solved analytically: the constant potential in a limited space [2], and the reflexionless potential in an unlimited space, which is treated here. It is shown that a reflexionless potential does not modify the spin polarization around the point field away from the range of the potential. This is not so, when there is a boundary. The spin polarization on the other side of the reflexionless potential is, however, modified.

A simple approximation is introduced based on a space dependent Fermi wave number. It agrees well with the exact result. Hopefully it can be used as a guideline in more general situations, when reflexions are not dominant.

APPENDIX: INTEGRATED POLARIZATION

In this appendix we shall generalize the result Eq. (36) to three dimensions and to a large class of potentials. We consider a non-interacting degenerate electron gas acted upon by a potential which is limited to a finite region in such a way that the wave functions with positive energy $\phi_{k,s}(\boldsymbol{x}) = \phi_k(x)\,\eta_s$ can be labeled by an incoming wave vector $\boldsymbol{k}$ and the spin quantum number $s = \pm\frac{1}{2}$, the energy being $\epsilon_k = \hbar^2 k^2/2m$. In addition there may be a discrete spectrum of bound states with wave functions $\phi_{n,s}(\boldsymbol{x}) = \phi_n(\boldsymbol{x})\,\eta_s$ and energies $\epsilon_n = -\hbar^2\lambda_n^2/2m$. The Fermi surface then is a sphere with radius k_F. A point field of strength γ at position $\boldsymbol{a}$ is coupled to the spins:

$$H' = -\gamma\,\delta(\boldsymbol{x}-\boldsymbol{a})\,\frac{\sigma_z}{2}. \tag{A1}$$

The resulting spin polarization of the electron gas $P(\boldsymbol{x},\boldsymbol{a})$ then satisfies

$$\mathcal{P}(\boldsymbol{a}) = \int d^3x\, P(\boldsymbol{x},\boldsymbol{a}) = \gamma\,\chi_P\,\left\langle|\phi_k(\boldsymbol{a})|^2\right\rangle_F, \tag{A2}$$

where χ_P is the Pauli susceptibility of the unperturbed electron gas, i.e. half the density of states per spin at the Fermi level, and $\left\langle|\phi_k(\boldsymbol{a})|^2\right\rangle_F$ is the average over the Fermi surface of the probability density of the wave function $\boldsymbol{k}$ at position $\boldsymbol{a}$. The wave functions of the continuum are normalized to a Dirac δ-function.

To calculate $P(\boldsymbol{x},\boldsymbol{a})$ in three dimensions we run through equations analogous to Eqs. (6) to (9) with additional terms if there are several bound states. However, the terms containing bound states vanish upon integration over $\boldsymbol{x}$, so that

$$\mathcal{P}(\boldsymbol{a}) = \int_{-\infty}^{\infty} P(\boldsymbol{x},\boldsymbol{a})\,d^3x \tag{A3}$$

$$= \frac{\gamma}{2}\,\frac{2m}{\hbar^2}\int_{-\infty}^{\infty}\frac{d^3k'}{(2\pi)^3}\int_{k\le k_F}\frac{d^3k}{(2\pi)^3}\int_{-\infty}^{\infty}d^3x\,\frac{\phi_k^*(\boldsymbol{x})\,\phi_{k'}^*(\boldsymbol{a})\,\phi_k(\boldsymbol{a})\,\phi_{k'}(\boldsymbol{x})}{k'^2-k^2} \;+\; \text{c.c.}. \tag{A4}$$

Using

$$\int_{-\infty}^{\infty} d^3x\, \phi_k^*(\boldsymbol{x})\, \phi_{k'}(\boldsymbol{x}) = (2\pi)^3\, \delta^3(\boldsymbol{k}-\boldsymbol{k}') \tag{A5}$$

and the change of variables $\boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{q}$ this becomes

$$\mathcal{P}(a) = \frac{\gamma}{2}\,\frac{2m}{\hbar^2} \int_{-\infty}^{\infty} \frac{d^3q}{(2\pi)^3}\, \delta^3(\boldsymbol{q}) \int_{k\le k_F} \frac{d^3k}{\boldsymbol{q}\cdot(2\boldsymbol{k}+\boldsymbol{q})} \left[\phi_{k+q}^*(\boldsymbol{a})\,\phi_k(\boldsymbol{a}) + \phi_{k+q}(\boldsymbol{a})\,\phi_k^*(\boldsymbol{a})\right]. \tag{A6}$$

In view of the δ–function only terms up to linear in q in the bracket must be retained. Thus

$$\mathcal{P}(a) = \frac{\gamma}{2}\,\frac{2m}{\hbar^2} \int_{-\infty}^{\infty} \frac{d^3q}{(2\pi)^3}\, \delta^3(\boldsymbol{q}) \int_{k\le k_F} \frac{d^3k}{\boldsymbol{q}\cdot(2\boldsymbol{k}+\boldsymbol{q})} \left[2|\phi_k(\boldsymbol{a})|^2 + \mathrm{grad}_k|\phi_k(\boldsymbol{a})|^2\cdot\boldsymbol{q}\right]. \tag{A7}$$

With the identity

$$\left(\mathrm{grad}_k|\phi_k|^2\right)\cdot\frac{\boldsymbol{q}}{2\boldsymbol{k}\cdot\boldsymbol{q}+q^2} = \mathrm{div}_k\left(|\phi_k|^2\frac{\boldsymbol{q}}{2\boldsymbol{k}\cdot\boldsymbol{q}+q^2}\right) + |\phi_k|^2\frac{2q^2}{(2\boldsymbol{k}\cdot\boldsymbol{q}+q^2)^2} \tag{A8}$$

$\mathcal{P}(\boldsymbol{a})$ can be written as a sum of two terms:

$$\mathcal{P}(\boldsymbol{a}) = G_1 + G_2 \tag{A9}$$

$$G_1 = \frac{\gamma}{2}\,\frac{2m}{\hbar^2} \int_{-\infty}^{\infty} d^3q\, \delta^3(\boldsymbol{q}) \int_{k\le k_F} \frac{d^3k}{(2\pi)^3} 2|\phi_k(\boldsymbol{a})|^2 \left[\frac{1}{2\boldsymbol{k}\cdot\boldsymbol{q}+q^2} + \frac{q^2}{(2\boldsymbol{k}\cdot\boldsymbol{q}+q^2)^2}\right] \tag{A10}$$

$$G_2 = \frac{\gamma}{2}\,\frac{2m}{\hbar^2} \int_{-\infty}^{\infty} d^3q\, \delta^3(\boldsymbol{q}) \int_{k\le k_F} \frac{d^3k}{(2\pi)^3}\, \mathrm{div}_k\left(|\phi_k(\boldsymbol{a})|^2\frac{\boldsymbol{q}}{2\boldsymbol{k}\cdot\boldsymbol{q}+q^2}\right). \tag{A11}$$

We shall show that $G_1 = 0$. This is somewhat delicate, since $\boldsymbol{q}$ cannot just be put equal to zero in the bracket. We invert the order of integrations and perform the angular integration of $\boldsymbol{q}$ first, using $\boldsymbol{k}$ as the polar axis. Using $\boldsymbol{k}\cdot\boldsymbol{q} = kq\cos\theta$ and

$$\delta^3(\boldsymbol{q})\, d^3q = \frac{1}{4\pi}\,\delta(q)\, dq\, d(\cos(\theta))\, d\phi \tag{A12}$$

G_1 becomes

$$G_1 = \frac{1}{2}\,\frac{\gamma}{2}\,\frac{2m}{\hbar^2} \int_{k\le k_F} \frac{d^3k}{(2\pi)^3}\, |\phi_k(\boldsymbol{a})|^2 \int_{-\infty}^{\infty} dq\, \delta(q) \left\{\frac{1}{2kq}\,\ln\left|\frac{q+2k}{q-2k}\right| + \frac{2}{q^2-4k^2}\right\}. \tag{A13}$$

The bracket vanishes for $q \to 0$.

G_2, Eq. (A11), is

$$G_2 = \frac{\gamma}{2}\,\frac{2m}{\hbar^2}\,k_F^2 \int_{-\infty}^{\infty} \frac{d^3q}{(2\pi)^3}\,\delta(\boldsymbol{q}) \int_{S_F} d\Omega_k |\phi_k(\boldsymbol{a})|^2 \frac{\boldsymbol{q}\cdot\hat{\boldsymbol{k}}}{2\boldsymbol{k}\cdot\boldsymbol{q}+q^2} \tag{A14}$$

$$= \frac{\gamma}{2}\,\frac{2m}{\hbar^2}\,\frac{k_F}{(2\pi)^2}\int_{S_F}\frac{d\Omega_k}{4\pi}|\phi_k(\boldsymbol{a})|^2, \tag{A15}$$

where S_F is the spherical Fermi surface, so that $d\boldsymbol{S} = k_F^2\, d\Omega_k\, \hat{\boldsymbol{k}}$, with the unit vector $\hat{\boldsymbol{k}}$. $\frac{k_F}{(2\pi)^2}\,\frac{2m}{\hbar^2}$ is the density of states per spin at the Fermi level. Hence Eq. (A15) coincides with Eq. (A2).

The corresponding result can also be established for one or two dimensional systems. Further explicit examples for these equations are given in [2] for infinite potentials outside a half space or a slab in one and in three dimensions. Actually the notation has to be adapted to these cases. For the slab in three dimensions the wave functions (Eq. (28) of [2]) are normalized as

$$\int dx \int d^2R\, \phi^*_{n,K}(x,\boldsymbol{R})\,\phi_{m,K'}(x,\boldsymbol{R}) = (2\pi)^2\,\delta(\boldsymbol{K}-\boldsymbol{K}')\,\delta_{n,m} \tag{A16}$$

Then the theorem reads

$$\mathcal{P}(a) = \frac{\gamma}{8\pi}\,\frac{2m}{\hbar^2} n_F\,\frac{1}{n_F}\sum_{n=1}^{n_F}\left\langle|\phi_{n,K}(a,0)|^2\right\rangle_{n,K_F} \tag{A17}$$

where $\left\langle|\phi_{n,K}(a,0)|^2\right\rangle_{n,K_F}$ is the average probability density of the wave functions which belong to n and to the Fermi energy, so that their $\boldsymbol{K}$ vector is situated on a circle of radius $K_F = \sqrt{k_F^2 - (n\pi/L)^2}$.

The Pauli susceptibility is obtained from the change in occupation due to the Zeeman shift in a homogeneous field. A point field modifies the wave functions and produces Zeeman shifts. The polarization, however, can be calculated from the changes of the wave functions alone, if the singularities are treated by principle part integration [10]. The integrated polarization represents the contribution of the point field to the Pauli susceptibility. The theorem states that this is obtained from the average Zeeman shift in the point field times the density of states.

FIGURES

FIG. 1. Spin polarization due to a point field at $a = 4$ in the presence of a potential well of strength $\lambda = 1$. Units are such that $k_F = 1$ and $\frac{\gamma}{4\pi}\frac{2m}{\hbar^2} = 1$. Lower dotted line: potential well in arbitrary units. Full line: spin polarization, Eq. (14). Stars: approximation with space dependent $k_F(x)$, Eq. (39). Dots: polarization in the absence of a potential well.

FIG. 2. Spin polarization due to a point field within the potential well. $a = -0.25$, $\lambda = 3$. Units and symbols as in Fig. 1.

FIG. 3. Spin polarization on one side of the potential well due to a point field on the opposite side ($a = -6$) for several strengths λ of the potential well. Full lines display the exact solutions, Eq. (14). The corresponding approximations, Eq. (39), are given by the following symbols: stars: $\lambda = 0$; squares: $\lambda = 0.5$; triangles: $\lambda = 1$; lozenges: $\lambda = 2$.

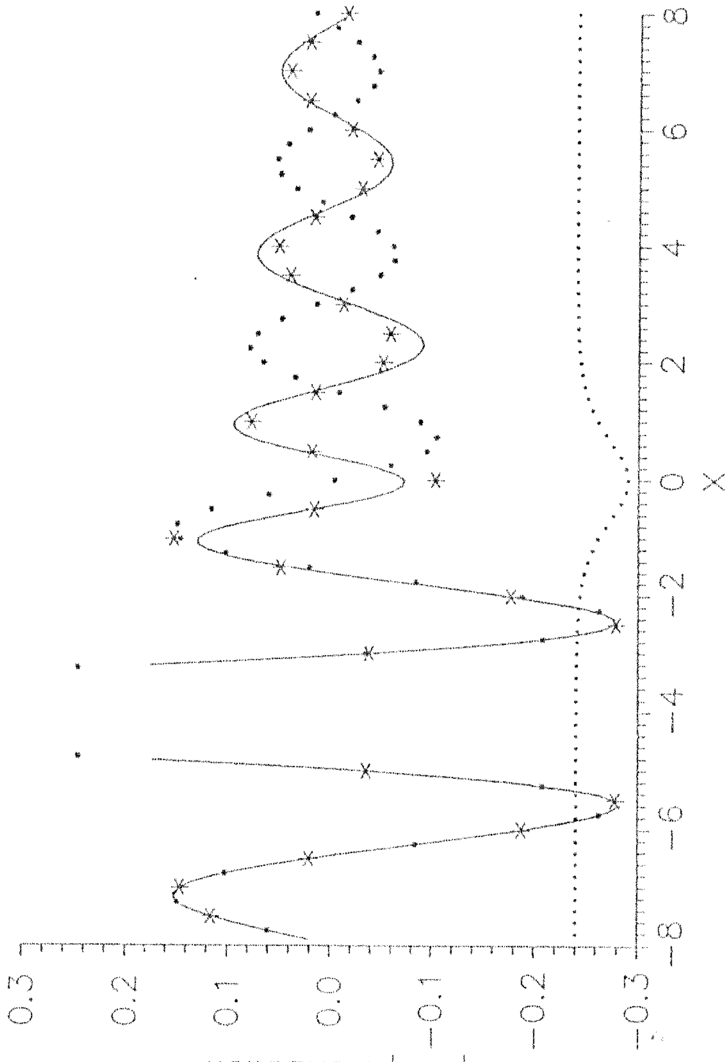

Figure 1

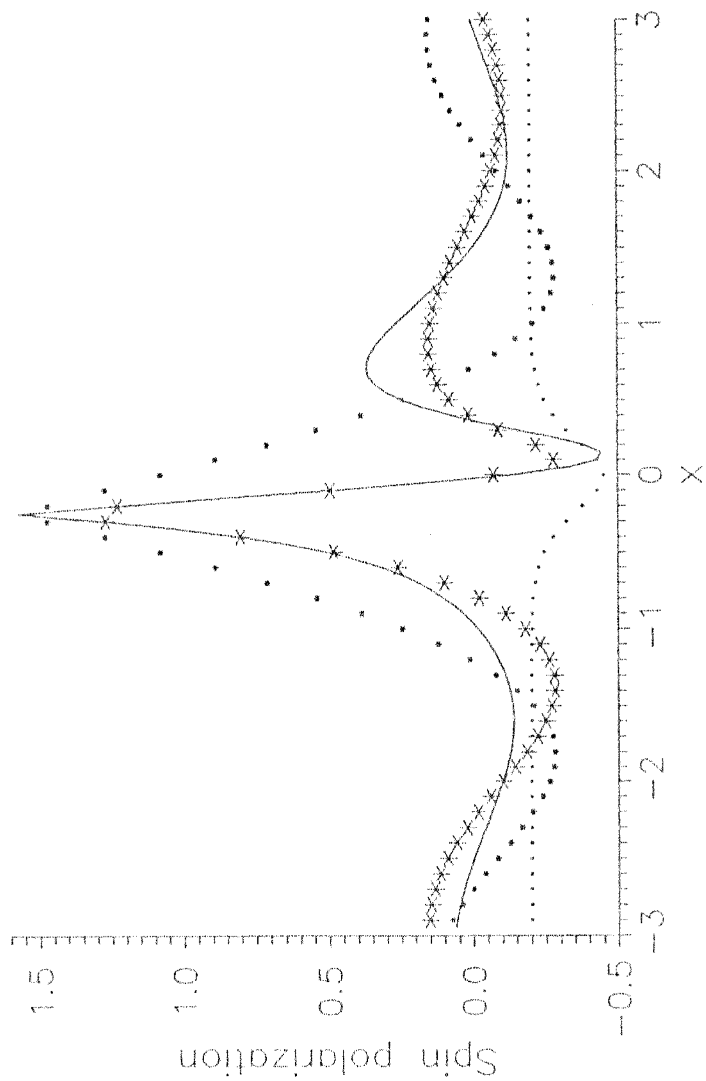

Figure 2

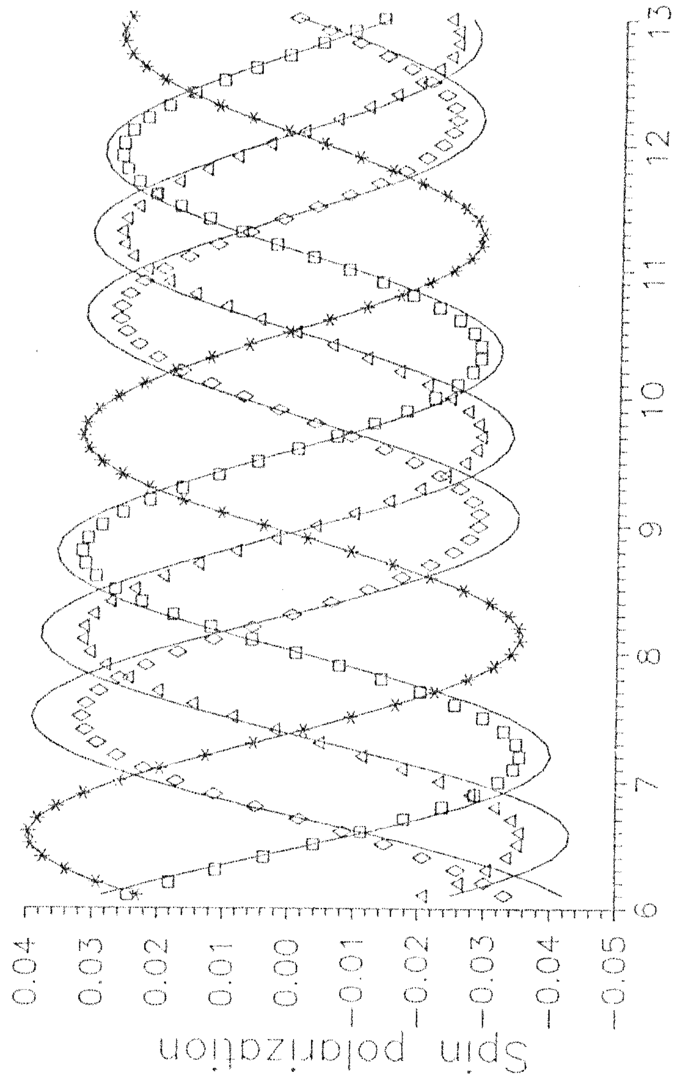
Spin polarization
X
0.04
0.03
0.02
0.01
0.00
−0.01
−0.02
−0.03
−0.04
−0.05
6
7
8
9
10
11
12
13

Figure 3

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