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Ruderman-Kittel-Kasuya-Yosida polarization in half-space and slab and in semi-infinite and finite lines

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Abstract

For a degenerate electron gas confined to a half-space or a slab the spin polarization produced by a point field is calculated. For the half-space both in three and one dimensions the analytic solution contains the usual RKKY polarization around the source plus a polarization wave originating from the mirror point, however, with the same phase at the border; there both are cancelled by a third term. In the slab the integrated polarization is finite, while it vanishes for the finite line.

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I. INTRODUCTION

Experiments with magnetic ions in limited metallic samples, such as films and layered structures have been of great interest recently. The question, how the RKKY [1] polarisation behaves in inhomogeneous media is relevant. Simple situations are those of a point ion spin in a half-space or in a slab in three and in one dimensions. This paper solves these problems to a large extent analytically. The model of a limited space is treated for simplicity; it does not pretend to represent all the complexities of real surfaces.

II. THE HALF-SPACE

Consider a fully degenerate ideal electron gas filling the half space $x > 0$. At the position $x = a,\ y = z = 0$, there is a point exchange field in the z direction acting on the spins of the electrons.

A complete set of one particle wave functions which vanish at the boundary $x = 0$ is given by

$$\phi_{k,K,s}(x, \boldsymbol{R}) = \sqrt{2}\sin(kx)\,\mathrm{e}^{iK\cdot R}|s\rangle, \tag{1}$$

where $k > 0$, $\boldsymbol{R} = (y, z)$, and $\boldsymbol{K} = (K_y, K_z)$. $|s\rangle$ represents the spin wave function for an electron with spin $s = \pm 1/2$ in the z-direction. The perturbing Hamiltonian is

$$H' = -\gamma\,\delta(x-a)\,\delta^2(\boldsymbol{R})\,\tfrac{\sigma_z}{2}, \tag{2}$$

where the coupling constant γ has the dimension energy·volume, and σ_z is the Pauli spin matrix for the z-direction. Yosida [2] has shown that the spin polarization which arises from the change in occupation connected with the Zeeman splitting of the levels can be ignored if the restriction not to include diagonal terms in the perturbed wave function is lifted. Thus we neglect the Zeeman splitting introduced by the perturbation, Eq. (2). The matrix elements of Eq. (2) are

$$\langle\phi_{k',K',s'}|H'|\phi_{k,K,s}\rangle = -2\gamma s\sin(ka)\,\sin(k'a)\,\delta_{s',s}. \tag{3}$$

The perturbed wave functions are

$$\psi_{k,K,s}(x,\boldsymbol{R}) = \phi_{k,K,s} - \frac{\sqrt{2}\,2\gamma s}{4\pi^3}\,\frac{2m}{\hbar^2}\int_0^\infty dk' \int_0^\infty dK'\,K' \int_0^{2\pi} d\varphi$$
$$\frac{\sin(ka)\sin(k'a)}{k^2+K^2-k'^2-K'^2}\sin(k'x)\,\mathrm{e}^{iK'R\cos(\varphi)}\,|s\rangle. \tag{4}$$

All the integrations can be performed analytically using $\int_0^\infty d\varphi\,\mathrm{e}^{iK'R\cos(\varphi)} = 2\pi\,J_0(K'R)$, where J_0 is the Bessel function of order zero, $\sin(k'x)\,\sin(k'a) = \frac{1}{2}[\cos(k'z_-) - \cos(k'z_+)]$ with $z_\mp = |x \mp a|$, and [3]

$$\int_0^\infty dk' \frac{\cos(k'z_\mp)}{C^2 - K'^2 - k'^2} = \begin{cases} \frac{\pi}{2}\frac{\sin\left(\sqrt{C^2-K'^2}z_\mp\right)}{\sqrt{C^2-K'^2}} & \text{for } C^2 > K'^2 \\ -\frac{\pi}{2}\frac{\exp\left(-\sqrt{K'^2-C^2}z_\mp\right)}{\sqrt{K'^2-C^2}} & \text{for } C^2 < K'^2 \end{cases} \tag{5}$$

with $C^2 = k^2 + K^2$, and [4]

$$\begin{aligned} - & \int_0^b dx\,x\,(b^2-x^2)^{-1/2}\sin\left(\alpha\sqrt{b^2-x^2}\right)J_0(xy) \\ + & \int_b^\infty dx\,x\,(x^2-b^2)^{-1/2}\exp\left(-\alpha\sqrt{x^2-b^2}\right)\,J_0(xy) \\ = & \quad (y^2+\alpha^2)^{-1/2}\cos\left(b\sqrt{y^2+\alpha^2}\right). \end{aligned} \tag{6}$$

The result is

$$\psi_{k,K,s} = \phi_{k.K,s} + \frac{\sqrt{2}}{8\pi}\,2\gamma s\,\frac{2m}{\hbar^2}\sin(ka)\left\{\frac{\cos\left(\sqrt{k^2+K^2}\rho_-\right)}{\rho_-} - \frac{\cos\left(\sqrt{k^2+K^2}\rho_+\right)}{\rho_+}\right\} \tag{7}$$

with $\rho_\mp = \sqrt{(x\mp a)^2 + R^2}$. The perturbation produces a superposition of two spherical waves, one of which originates at the position $(a,0,0)$, and the other at the mirror point $(-a,0,0)$.

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

$$P_h(x,\boldsymbol{R}) = \int_{\text{occupied states}} \tfrac{dk\,d^2K}{4\pi^3}\sum_s \psi^*_{k,K,s}(x,\boldsymbol{R})\,\tfrac{1}{2}\sigma_z\,\psi_{k,K,s}(x,\boldsymbol{R}), \tag{8}$$

where the sum extends over states with $k^2 + \boldsymbol{K}^2 < {k_F}^2$, with k_F, the Fermi wave number.

$$P_h(x,\boldsymbol{R}) = \frac{1}{2^5\pi^4}\,\gamma\,\frac{2m}{\hbar^2}\int_0^{k_F} dk \int_0^{\sqrt{k_F^2-k^2}} dK\,K \int_0^{2\pi} d\varphi\,\sin(kx)\,\sin(ka)$$
$$\cdot\,\mathrm{e}^{iKR\cos(\varphi)}\left\{\frac{\cos\left(\sqrt{k^2+K^2}\rho_-\right)}{\rho_-} - \frac{\cos\left(\sqrt{k^2+K^2}\rho_+\right)}{\rho_+}\right\} \quad + \quad \text{c.c.} \tag{9}$$

Once more these integrals can be performed analytically. We obtain

$$P_h = \frac{\gamma}{8\pi^3}\frac{2m}{\hbar^2}\left[I_{--} - I_{-+} - I_{+-} + I_{++}\right], \tag{10}$$

where the two indices refer to the index of $z_\mp$ and $\rho_\mp$ in integrals like

$$I_{-+} = \int_0^{k_F} dk \int_0^{\sqrt{k_F^2-k^2}} dK\, K\, J_0(KR)\, \cos(kz_-)\frac{\cos(\sqrt{k^2+K^2}\rho_+)}{\rho_+}. \tag{11}$$

With $K = q\sin(\theta), \quad k = q\,\cos(\theta), \quad dk\,dK = q\,dq\,d\theta$

$$I_{-+} = \int_0^{k_F} dq\, q^2\, \frac{\cos(q\rho_+)}{\rho_+} \int_0^{\pi/2} d\theta\, \sin(\theta)\, J_0(qR\sin(\theta))\, \cos(qz_-\,\cos(\theta)). \tag{12}$$

which becomes [5]

$$I_{-+} = \int_0^{k_F} dq\, q\, \frac{\cos(q\rho_+)}{\rho_+\rho_-}\sin(q\rho_-). \tag{13}$$

The remaining integrals are elementary. The final result can be expressed with the RKKY-function

$$R(x) = \frac{\gamma k_F^4}{4\pi^3}\frac{2m}{\hbar^2}\,\frac{\sin(x) - x\cos(x)}{x^4} \tag{14}$$

as

$$P_h = R(2k_F\rho_-) + R(2k_F\rho_+) - \frac{(\rho_- + \rho_+)^2}{2\rho_-\rho_+}\, R(k_F(\rho_- + \rho_+)). \tag{15}$$

The first term is the usual RKKY polarization in infinite space. The second term corresponds to a reflected wave originating from the mirror point $(-a, 0, 0)$. The third term compensates the first two terms at the boundary and is of the same order as the others in the whole half space. See Figs. 1 and 2.

The RKKY polarization in thin wires has been discussed [6] with the method of Feynman path integration, where, however, only direct and reflected waves appear.

The existence of a direct wave and of a reflected wave in $P_h(x, \boldsymbol{R})$ could be expected. The fact is, however, that the magnetic polarizations belonging to the two waves are equal at the surface. They do not compensate each other. Since the total polarization at the surface, where the electron density vanishes, must be zero, a third term which compensates the two previous terms becomes unavoidable. This third term extends over the whole space with similar amplitudes as the other two terms.

III. INTEGRATED POLARIZATION IN THE HALF-SPACE

The integrated polarization as a function of the position a of the source

$$\mathcal{P}(a) = \int_{\text{half space}} d^3r \, P_h(x, \boldsymbol{R}) \tag{16}$$

is an important quantity. The integral over the first two terms in Eq. (15) add up to the integral over the first in infinite space

$$\int d^3x \, R(2k_F\rho_-) = \frac{\gamma k_F}{8\pi^2}\frac{2m}{\hbar^2}. \tag{17}$$

For the third term elliptic coordinates are adequate. The rotational ellipsoid with half axes A and B

$$\frac{x^2}{A^2} + \frac{y^2+z^2}{B^2} = 1 \tag{18}$$

allows the parametrization

$$x = \quad A\,\cos(\varphi) \tag{19}$$

$$y = B\,\sin(\varphi)\,\cos(\psi) \tag{20}$$

$$z = B\,\sin(\varphi)\,\sin(\psi). \tag{21}$$

Here $B = \sqrt{A^2 - a^2}$, where the focal distance a is the position of the point field. The excentricity $\epsilon = a/A$ is connected with the two radii by

$$\rho_1 = A + \epsilon\, x, \qquad \rho_2 = A - \epsilon\, x. \tag{22}$$

The Jacobian J of the transformation, $dx\,dy\,dz = J\,da\,d\varphi\,d\psi$ becomes $J = \sin(\varphi)\,[A^2 - a^2\cos^2(\varphi)]$. Then $J\,(\rho_1+\rho_2)^2/(\rho_1\rho_2) = (2A)^2\sin(\varphi)$, so that

$$\int_0^\infty dA \int_0^{\pi/2} d\varphi \int_0^{2\pi} d\psi\, \sin(\varphi)\,(2A)^2 R(2k_F A) = \frac{\gamma k_F}{8\pi^2}\frac{2m}{\hbar^2}\,\frac{\sin(2k_F a)}{2k_F a}. \tag{23}$$

Thus

$$\mathcal{P}(a) = \frac{\gamma k_F}{8\pi^2}\,\frac{2m}{\hbar^2}\left[1 - \frac{\sin(2k_F a)}{2k_F a}\right]. \tag{24}$$

With distance there is a oscillatory behaviour with decreasing amplitude. The overshooting or suppression of the polarization depends on how the RKKY oscillations fit into the distance between the source and the surface. The average of the probability density of the wave functions on the Fermi surface S_F is

$$\langle|\phi_{k,K,s}(a,0)|\rangle_{S_F} = \frac{1}{4\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \, \sin(\theta)\, 2\, \sin^2(k_F a\, \cos(\theta) \tag{25}$$

$$= \qquad 1 - \frac{\sin(2k_f a)}{2k_F a}. \tag{26}$$

Eq. (24) combined with Eq. (26) is a special case of a general theorem [7].

A integral over a gives the integrated polarization from a homogeneous field. Since

$$\int_0^\infty \frac{\sin(2k_F a)}{2k_F a} = \frac{\pi}{4k_F} = \frac{\lambda_F}{8} \tag{27}$$

with $k_F = 2\pi/\lambda_F$, the integrated Pauli susceptibility of a half space is reduced near the surface as if a slab of width $\lambda_F/8$ were missing.

IV. THE SLAB

For a slab or film of thickness L the boundary condition that the wave functions vanish for $x = 0$ and $x = L$ is assumed. We thus use the complete set of wave functions

$$\varphi_{n,\mathbf{K},\mathbf{s}}(x,\mathbf{R}) = \sqrt{\frac{2}{L}}\, \sin\left(\frac{n\pi x}{L}\right) \mathrm{e}^{i\mathbf{K}\cdot\mathbf{R}}, \qquad n = 1,2,\ldots. \tag{28}$$

The perturbed wave function becomes

$$\chi_{n,\mathbf{K},\mathbf{s}}(x,\mathbf{R}) = \varphi_{n,\mathbf{K},\mathbf{s}} - \frac{\sqrt{2}\,2\gamma s}{(2\pi)^2 L^{3/2}} \frac{2m}{\hbar^2} \sum_{n'=1}^{\infty} \int_0^\infty dK'\, K' \int_0^{2\pi} d\varphi$$
$$\cdot \frac{\sin(n\pi a/L)\, \sin(n'\pi a/L)}{(n\pi/L)^2 + K^2 - (n'\pi/L)^2 - K'^2} \sin(n'\pi x/L) \mathrm{e}^{iK'R\cos(\varphi)}\, |s\rangle. \tag{29}$$

The sum over n' can be performed with the aid of Poisson's formula [8] which yields for $D > 0$:

$$\frac{1}{2D^2} + \sum_{n=1}^{\infty} \frac{\cos(nC)}{D^2 - n^2} = \frac{\pi}{2} \sum_{n=-\infty}^{\infty} \frac{\sin(D|C + 2\pi n|)}{D} \tag{30}$$

$$\frac{1}{2D^2} + \sum_{n=1}^{\infty} \frac{\cos(nC)}{D^2 + n^2} = \frac{\pi}{2}\frac{1}{D} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-D|C+2\pi n|}. \tag{31}$$

We can again use Eq. (6) for the integration over K'. With the dimensionless quantities

$$Q = \sqrt{n^2 + (KL/\pi)^2}, \qquad \rho_{l,\pm} = \frac{\pi}{L}\sqrt{R^2 + (|x \pm a| + 2lL)^2} \tag{32}$$

the wave function Eq. (29) becomes

$$\begin{aligned} \chi_{n,\mathbf{K},s}(x,\mathbf{R}) = & \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \mathrm{e}^{i\mathbf{K}\cdot\mathbf{R}} \\ & + \frac{\sqrt{2}}{8L^{3/2}} 2\gamma s \frac{2m}{\hbar^2} \sin\left(\frac{n\pi a}{L}\right) \sum_{l=-\infty}^{\infty} \left[\frac{\cos(Q\rho_{l,-})}{\rho_{l,-}} - \frac{\cos(Q\rho_{l,+})}{\rho_{l,+}}\right]. \end{aligned} \tag{33}$$

The polarization now reads

$$P_f(x,\mathbf{R}) = \sum_{\substack{n \\ \text{occupied states}}} \int \frac{d^2K}{(2\pi)^2} \sum_s \chi^*_{n,\mathbf{K},s}(x,\mathbf{R}) \frac{\sigma_z}{2} \chi_{n,\mathbf{K},s}(x,\mathbf{R}). \tag{34}$$

Which are the occupied states? Let ϵ_F be the energy of the highest occupied level. It corresponds to a wave number k_F through $\epsilon_F = \hbar^2 k_F^2/(2m)$. The x-component of the wave vector is quantized as $\pi n/L$, while the y- and z-components are continuous. We call n_F the highest value of n for which occupied states exist. Both n_F and k_F are determined by the total electron density N. They must reproduce the number of electrons per unit surface of the slab through

$$\frac{NL}{2} = \sum_{n=1}^{n_F} \int_0^{\sqrt{k_F^2-(\pi n/L)^2}} \frac{2\pi K\,dK}{(2\pi)^2} = \frac{1}{4\pi} \sum_{n=1}^{n_F} \left\{k_F^2 - \left(\frac{\pi n}{L}\right)^2\right\} \tag{35}$$

$$\frac{2}{\pi} N L^3 = n_F \left(\frac{L k_F}{\pi}\right)^2 - \frac{1}{6} n_F (n_F+1)(2n_F+1) \tag{36}$$

and fulfill the relation

$$n_F \le k_F L/\pi < n_F + 1. \tag{37}$$

n_F counts the number of half waves within the thickness L of the slab. The Eqs. (36) and (37) yield unambigously n_F and k_F. For $n_F \gg 1$ they lead to $n_F \approx k_F L/\pi$ with $k_F = (3\pi^2 N)^{1/3}$, so that $n_F^3 \approx (3/\pi) N L^3$. k_F and the energy as functions of N are different analytical expressions for each value of $n_F(N)$; numerically, however, the two functions are remarkably smooth.

Now Eq. (34) becomes

$$P_f(x,\mathbf{R}) = \frac{\pi}{4L^4}\,\gamma\,\frac{2m}{\hbar^2}\sum_{n=1}^{n_F}\sin\left(\frac{n\pi a}{L}\right)\,\sin\left(\frac{n\pi x}{L}\right)\,\sum_{l=-\infty}^{\infty}(I_{l,-}-I_{l,+}), \tag{38}$$

where the indexes $l,-$ or $l,+$ refer to those of ρ.

$$I_{l,\pm} = \frac{1}{\rho_{l,\pm}}\int_0^{\sqrt{(k_F L/\pi)^2-n^2}} dz\, z\, J_0(\frac{z\pi R}{L})\,\cos(\sqrt{z^2+n^2}\rho_{l,\pm}) \tag{39}$$

where $z = KL/\pi$.

On the axis, $\mathbf{R}=0$, the integral Eq. (39) can be performed analytically, yielding

$$I_{l,\pm} = \frac{1}{\rho_{l,\pm}^3}\left[f_1\left(\frac{k_F L}{\pi}\rho_{l,\pm}\right) - f_1\left(n\rho_{l,\pm}\right)\right] \tag{40}$$

with $f_1(x) = \cos(x) + x\sin(x)$. The infinite sum in Eq. (38) converges quickly, because for large l the difference $I_{l,-}-I_{l,+}$ is proportional to l^{-3}. $P_f(x,R)2k_F|x-a|$ is plotted in Fig. 3.

V. INTEGRATED POLARIZATION IN THE SLAB

To calculate the integral of the polarization over the volume of the slab as a function of a, it is convenient to write the polarization using Eq. (29) for the wave function.

$$P_f(x,\boldsymbol{R}) = -\sum_{\substack{n \\ \text{occupied states}}}\int d^2K\,\frac{2}{L^2}\,\gamma\,\frac{2m}{\hbar^2}\,\frac{1}{(2\pi)^4}\sum_{n'=1}^{\infty}\int d^2K'\frac{\sin\left(\frac{n\pi a}{L}\right)\,\sin\left(\frac{n'\pi a}{L}\right)}{(\pi/L)^2(n^2-n'^2)+K^2-K'^2}$$
$$\cdot\sin\left(\frac{n\pi x}{L}\right)\,\sin\left(\frac{n'\pi x}{L}\right)\,\mathrm{e}^{i(K-K')\cdot R} + \text{ c.c.}, \tag{41}$$

where the integration over $\boldsymbol{K}'$ extends over the whole space. The integration over x leads to

$$\mathcal{P}(\boldsymbol{R}) = \int_0^L P_f(x,\boldsymbol{R})\,dx = \frac{-1}{(2\pi)^4 L}\,\gamma\,\frac{2m}{\hbar^2}\sum_{\substack{n \\ \text{occupied states}}}\int d^2K\,\sin^2\left(\frac{n\pi a}{L}\right)\int d^2K'\frac{\mathrm{e}^{i(K-K')\cdot R}}{K^2-K'^2} + \text{ c.c.}. \tag{42}$$

With $\boldsymbol{q} = \boldsymbol{K}-\boldsymbol{K}'$ Eq. (42) becomes

$$\mathcal{P}(\boldsymbol{R}) = \frac{\gamma}{L}\,\frac{2m}{\hbar^2}\sum_{n=1}^{n_F}\sin^2\left(\frac{n\pi a}{L}\right)\int\frac{d^2q}{(2\pi)^2}\,\mathrm{e}^{iq\cdot R}\int_0^{\sqrt{k_F^2-(n\pi/L)^2}}\int_0^{2\pi}d\varphi\frac{2}{q^2-4K^2\cos^2(\varphi)}. \quad (43)$$

These integrals can be performed analytically. The integrals over φ and K were considered by Kittel [9] in the evaluation of the spin susceptibility in two dimensions. The result is

$$\mathcal{P}(\boldsymbol{R}) = \frac{\gamma}{4L}\,\frac{2m}{\hbar^2}\sum_{n=1}^{n_F}\sin^2\left(\frac{n\pi a}{L}\right)\int\frac{d^2q}{(2\pi)^2}\,\mathrm{e}^{iq\cdot R}\chi_0(q,n), \quad (44)$$

where

$$\chi_0(q,n) = \frac{1}{\pi}\left\{\Theta(2k_{Fn}-q) + \left[1-\sqrt{1-(k_{Fn}/q)^2}\right]\,\Theta(q-2k_{Fn})\right\} \quad (45)$$

with $k_{Fn} = \sqrt{k_F^2-(n\pi/L)^2}$ and Θ the step function.

The Fourier transform in Eq (44) was performed by Béal-Monod [10]. The result is

$$\mathcal{P}(R) = \frac{\gamma}{4L}\,\frac{2m}{\hbar^2}\sum_{n=1}^{n_F}\sin^2\left(\frac{n\pi a}{L}\right)\tilde{\chi}_0(R,n) \quad (46)$$

$$\tilde{\chi}_0(R,n) = -\frac{k_{Fn}^2}{2\pi}\left[J_0(k_{Fn}R)\,N_0(k_{Fn}R) - J_1(k_{Fn}R)\,N_1(k_{Fn}R)\right]. \quad (47)$$

The spacial integration over $\boldsymbol{R}$ is immediate from Eq. (44)

$$p(a) = \int d^2R\,\mathcal{P}(\boldsymbol{R}) = \frac{\gamma}{8\pi}\,\frac{2m}{\hbar^2}\,n_F\,\frac{2}{Ln_F}\sum_{n=1}^{n_F}\sin^2\left(\frac{n\pi a}{L}\right). \quad (48)$$

A further integration over a

$$\int_0^L da\,p(a) = \frac{\gamma}{8\pi}\,\frac{2m}{\hbar^2}\,n_F \approx \frac{\gamma k_F L}{8\pi^2}\,\frac{2m}{\hbar^2} \quad (49)$$

reproduces the Pauli susceptibility in the limit of $k_F L/\pi \gg 1$.

VI. SUSCEPTIBILITY IN RECIPROCAL SPACE

Eq. (41) may be written in terms of a generalized susceptibility $\chi(q,n,n')$ as

$$P_f(x,\boldsymbol{R}) = \frac{\gamma}{2L^2}\frac{2m}{\hbar^2}\sum_{n=1}^{n_F}\sum_{n'=1}^{\infty}\sin\left(\frac{n\pi}{l}a\right)\,\sin\left(\frac{n'\pi}{L}a\right)\,\sin\left(\frac{n\pi}{L}x\right)\,\sin\left(\frac{n'\pi}{L}x\right) \cdot\int\frac{d^2q}{(2\pi)^2}\,\mathrm{e}^{iq\cdot R}\chi(q,n,n'), \quad (50)$$

where

$$\chi(q,n,n') = -\frac{D}{\pi q^2}\left\{\Theta(W^2-1) + (1-\sqrt{1-W^2})\,\Theta(1-W^2)\right\} \tag{51}$$

with $W = 2qk_F/D, \quad D = (\pi/L)^2(n^2 - n'^2) - q^2$. Note that when Eq. (50) is integrated over $\boldsymbol{x}$ in the interval $\{0, L\}$ it coincides with Eq. (44).

VII. THE HALF-LINE

The program of finding the spin polarisation due to a point field in limited spaces, which was carried out in the preceding sections, can be performed analytically to the end in the one dimensional case. This may apply to mesoscopic wires which are sufficiently thin so that the side motion is frozen out by the quantum size effect.

Set of wave functions for the half-line:

$$\phi_{k,s}(x) = \sqrt{2}\sin(kx)|s\rangle. \tag{52}$$

Perturbing Hamiltonian:

$$H' = -\gamma\,\delta(x-a)\,\tfrac{1}{2}\sigma_z. \tag{53}$$

As pointed out in section 2, Yosida [2] has shown that the correct polarization can be obtained from the first order perturbation of the wave function alone, if the sums over continuous states include the diagonal term. We shall again follow this prescription in the treatment of the half-line. Matrix element:

$$\langle\phi_{k',s'}|H'|\phi_{k,s}\rangle = -2\gamma s\,\sin(ka)\,\sin(k'a)\,\delta_{s,s'}. \tag{54}$$

Perturbed wave function:

$$\begin{aligned}\psi_{k,s}(x) &= \phi_{k,s}(x) - \sqrt{2}\gamma s\,\sin(ka)\,\frac{2m}{\hbar^2}\int_0^\infty \frac{dk'}{\pi}\frac{\cos\left(k'(x-a)\right) - \cos\left(k'(x+a)\right)}{k^2 - k'^2}|s\rangle \\ &= \phi_{k,s}(x) - \frac{\sqrt{2}\gamma s}{2k}\,\frac{2m}{\hbar^2}\,\sin(ka)\left[\sin\left(k|x-a|\right) - \sin\left(k(x+a)\right)\right]|s\rangle. \end{aligned}\tag{55}$$

Polarization:

$$\begin{aligned}
P_{1h}(x) &= \sum_s \int_0^{k_F} \frac{dk}{\pi} \psi^*_{k,s}(x)\, \frac{1}{2}\sigma_z\, \psi_{k,s}(x) && (56)\\
&= -\frac{1}{2\pi}\gamma\, \frac{2m}{\hbar^2} \int_0^{k_F} \frac{dk}{k} \left[\cos\left(k|x-a|\right) - \cos\left(k(x+a)\right)\right] \\
&\qquad \cdot \left[\sin\left(k|x-a|\right) - \sin\left(k(x+a)\right)\right] && (57)\\
&= -\frac{\gamma}{4\pi}\, \frac{2m}{\hbar^2} \left[\mathrm{Si}\left(2k_F|x-a|\right) + \mathrm{Si}\left(2k_F(x+a)\right) - 2\,\mathrm{Si}\left(k_F(|x-a|+x+a)\right)\right]. && (58)
\end{aligned}$$

In the unlimited one dimensional space the spin polarization is [11]:

$$R_1(|x-a|) = \frac{\gamma}{4\pi}\, \frac{2m}{\hbar^2} \left[\frac{\pi}{2} - \mathrm{Si}(2k_F|x-a|)\right]. \tag{59}$$

Thus

$$P_{1h}(x) = R_1(|x-a|) + R_1(x+a) - 2R_1\left(\frac{|x-a|+x+a}{2}\right). \tag{60}$$

The last term compensates the first two for $x=0$. The structure of the formula for $P_{1h}(x)$ is analogous to the 3 dimensional case. $P_{1h}(x)$ is plotted in Fig. 4.

The question of the order of the integrations and the contribution of the singularity at $k=k'=0$ has been a dominant theme in the treatment of the spin susceptibility in unlimited, homogeneous media [2] [11]. The constant term $\pi/2$ in Eq. (59) arises from this singularity [11]. However, in Eq. (60) this term cancels out. In the one dimensional half-space these questions are not relevant; the wave function Eq. (52) does not even exist for $k=0$.

VIII. INTEGRATED POLARIZATION OF HALF-LINE

It is interesting to evaluate the integrated polarization produced by the point interaction, Eq. (53). In unlimited space it is

$$\int_{-\infty}^{\infty} R_1(|x-a|)\, dx = \frac{\gamma}{4\pi k_F}\, \frac{2m}{\hbar^2}. \tag{61}$$

In the one-dimensional half-space the integration becomes

$$\int_0^\infty dx\, P_{1h}(x) = \frac{\gamma}{4\pi k_F}\,\frac{2m}{\hbar^2}\,\{1-\cos(2k_F a)\}\,. \tag{62}$$

The result oscillates with the position a of the point field. Eq. (62) also follows from a general theorem [7]. An integration of Eq. (62) over the position a gives the total spin produced by a homogeneous field of strength γ. This integral is not properly defined; as a function of the limit of integration it oscillates indefinitely around the mean value $\gamma\cdot(2m/\hbar^2)/(4\pi k_F)\cdot$Volume, which corresponds to the Pauli susceptibility.

IX. THE FINITE LINE

The wave functions vanish at the limits of the interval $0 \le x \le L$. A normalized set of functions are

$$\varphi_{n,s}(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi n x}{L}\right)\,|s\rangle, \qquad n = 1, 2, \ldots\,. \tag{63}$$

Now the wave numbers are discreet. In this case the prescription of Yosida [2] does not apply; the normal rules of perturbation theory must be followed. First the perturbation, Eq. (53), must be diagonalized within the degenerate spin states. The resulting energies are

$$\epsilon_{n,s} = \frac{\hbar^2\pi^2}{2mL^2}\,n^2 - \frac{2\gamma}{L}s\sin^2\left(\frac{n\pi a}{L}\right). \tag{64}$$

Between the levels n, s and $n+1, s$ there is a gap $\Delta\epsilon_{n,s} = (2n+1)\hbar^2\pi^2/(2mL^2)$. While $\Delta\epsilon_{n_F,s} > |\gamma|/L$ and $k_B T \ll \Delta\epsilon_{n_F,s}$, where T is the temperature, there is no change of occupation. Here n_F is the highest occupied number n. Multiplying the first inequality by n_F, the left side becomes larger than twice the Fermi energy, while the right side is $|\gamma|$ times the density of electrons of one spin. In three dimensions this is typically of the order of 0.3 eV, while $2\epsilon_{n_F,s}$ is of the order 10 eV. We shall assume that L is sufficiently small, so that there is no change of occupation. In the denominators of the second order perturbation theory the spin dependent parts of the energy cancel out.

With Eq. (53) the perturbed wave function becomes

$$\chi_{n,s}(x) = \varphi_{n,s}(x) - \gamma s\sqrt{\frac{2}{L^3}}\,\frac{2m}{\hbar^2}\sin\left(\frac{n\pi a}{L}\right)$$
$$\cdot \sum_{m=1}^{\infty}{}' \frac{\cos((m\pi/L)|x-a|) - \cos((m\pi/L)(x+a))}{(\pi^2/L^2)\,(n^2-m^2)}\,|s\rangle, \tag{65}$$

where the sum excludes the term $m = n$. For non integer n the sum over all integers m is known [12]. The restricted sum for integer n can be obtained as a limiting value

$$\sum_{m=1}^{\infty}{}' \frac{\cos(mC)}{n^2-m^2} = \lim_{\delta\to 0}\left\{\sum_{m=1}^{\infty}\frac{\cos(mC)}{(n+\delta)^2-m^2} - \frac{\cos(nC)}{(n+\delta)^2-n^2}\right\} \tag{66}$$
$$= -\frac{2+\cos(nC)}{4n^2} + \frac{\sin(nC)\,(\pi-C)}{2n}. \tag{67}$$

With

$$A = (\pi/L)\,|x-a|, \qquad B = (\pi/L)\,(x+a) \tag{68}$$

Eq. (65) becomes

$$\chi_{n,s} = \varphi_{n,s} + \sqrt{\frac{2}{L^3}}\,\frac{\gamma s L^2}{4\pi^2}\,\frac{2m}{\hbar^2}\sin\left(\frac{n\pi a}{L}\right)\left[\frac{\cos(nA)}{n^2} - 2(\pi-A)\frac{\sin(nA)}{n}\right.$$
$$\left. - \frac{\cos(nB)}{n^2} + 2(\pi-B)\frac{\sin(nB)}{n}\right]\,|s\rangle. \tag{69}$$

Let n_F denominate the highest doubly occupied level, so that $n_F = \mathrm{Int}(N/2)$ with N the number of electrons. Then these doubly occupied levels give a spin polarization

$$P_{1f}(x) = \sum_{n=1}^{n_F}\sum_{s}\chi^*_{n,s}(x)\,\frac{1}{2}\sigma_z\,\chi_{n,s}(x). \tag{70}$$

It can be written conveniently in terms of the function

$$Q(y) = \gamma\,\frac{2m}{\hbar^2}\sum_{n=1}^{n_F}(\cos(ny) + n(2\pi-y)\,\sin(ny))\frac{1}{n^2} \tag{71}$$

as

$$P_{1f}(x) = \frac{1}{8\pi^2}\{2Q(A+B) + Q(A-B) + Q(B-A) - Q(2A) - Q(2B) - 2Q(0)\}. \tag{72}$$

which is plotted in Fig. 4.

In a one dimensional system n_F need not be a large number, and the question arises, whether the number of electrons is even or odd. Between the unperturbed levels n and

$n+1$ there is an energy gap of value $(\hbar^2/2m)(\pi/L)^2(2n+1)$. The above results Eqs. (71) and (72) give the full polarization when each level is doubly occupied. If a further level $\tilde{n} = n_F + 1$ is singly occupied, the lower Zeeman split level gives a contribution to Eq. (72) as

$$\phi^*_{\tilde{n},s}\,\tfrac{1}{2}\sigma_z\,\phi_{\tilde{n},s} + 2\phi^*_{\tilde{n},s}\,\tfrac{1}{2}\sigma_z\,(\chi_{\tilde{n},s} - \phi_{\tilde{n},s}). \tag{73}$$

The first term gives the first order contribution of the unpaired spin. The second term of (73) adds to $Q(y)$ half a term with $n = \tilde{n}$.

For finite L the integral over the polarization $\int_0^L dx\, P_{1f}(x)$ vanishes. This can be seen by an actual integration, which is elementary, but involves detailed considerations of the ranges of integration for the various terms due to the presence of absolute value functions. The result is expected, since P_{1f} describes the polarization from doubly occupied levels separated by energy gaps. An additional electron in a singly occupied level has a polarization of which the first term of Eq. (73) integrates to one spin.

For a comparison with the results from the half-line, Eqs. (59) and (60), we let L go to infinity so that $k_F = \pi N/(2L)$ remains constant. Then

$$\sum_{n=1}^{n_F} \frac{\sin(nx\pi/L)}{n} \;\Rightarrow\; \int_0^{k_F x} \frac{\sin(y)}{y} dy = \mathrm{Si}(k_F x) \tag{74}$$

and

$$\sum_{n=1}^{k_F L/\pi} \frac{\cos(nx\pi/L)}{n^2} \;\Rightarrow\; \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}. \tag{75}$$

In this limit Eq. (72) coincides with Eq. (60). Obviously, the two quantities $\lim_{L\to\infty} \int_0^L dx\, P_{1f}(x)$ and $\int_0^\infty dx\, \lim_{L\to\infty} P_{1f}(x)$ are not equal, since the first vanishes, while the second is given by Eq. (62). The fact that $\lim_{L\to\infty} P_{1f}(x) = P_{1h}(x)$, which contains the Pauli susceptibility, is the essence of Yosida's [2] remark, that the principle value integral of the energy denominators yields the "$q = 0$" term.

FIGURES

FIG. 1. Polarization $P_h(x,R)\,\rho_-$ due to a point field at $a=4$. The factor ρ_-, which is the distance to the point source, suppresses the divergence of P_h at the source and emphasizes the oscillations. The polarization vanishes at the surface $x=0$. Distances are in units of $1/(2k_F)$ and P_h is in units of $\gamma k_F^4\, 2m/(4\pi^3\hbar^2)$.

FIG. 2. $P_h(x,R)\,\rho_-$ is plotted along the x-axis and, for increasing R, in a direction perpendicular to the x-axis. Full line: $P_h(x,0)\,\rho_-$ versus x; dashed line: $P_h(a,R)\,\rho_-$ versus $R+a$. The dotted line shows the RKKY function $R(|x-a|)\,|x-a|$ for comparison. $a=4$, units as in Fig. 1.

FIG. 3. $P_f(x,R)\,\rho_-$ is plotted along the x-axis and, for increasing R, in a direction perpendicular to the x-axis. Full line: $P_f(x,0)\,\rho_-$ versus x; dashed line: $P_f(a,R)\,\rho_-$ versus $R+a$. Dotted line: the RKKY function $R(|x-a|)\,|x-a|$ is shown for comparison. $a=4$, $L=32$, units as in Fig. 1.

FIG. 4. Polarizations in one dimension. Dashed line: $P_{1h}(x)$; full line: $P_{1f}(x)$; dotted line: the RKKY function $R1(|x-a|)$. $a=4$, $L=32$, $n_F=5$. Distances are in units of $1/(2k_F)$ and polarizations in units of $\frac{\gamma}{4\pi}\,\frac{2m}{\hbar^2}$.

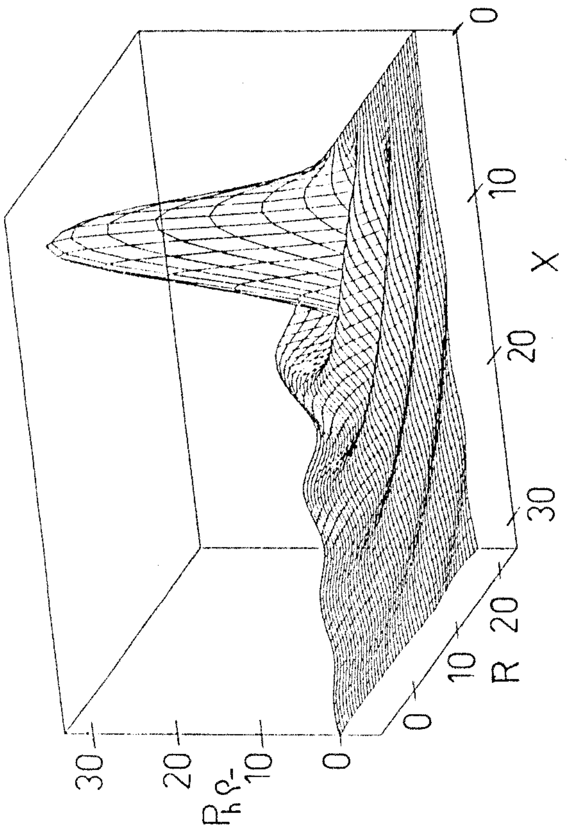

Figure 1

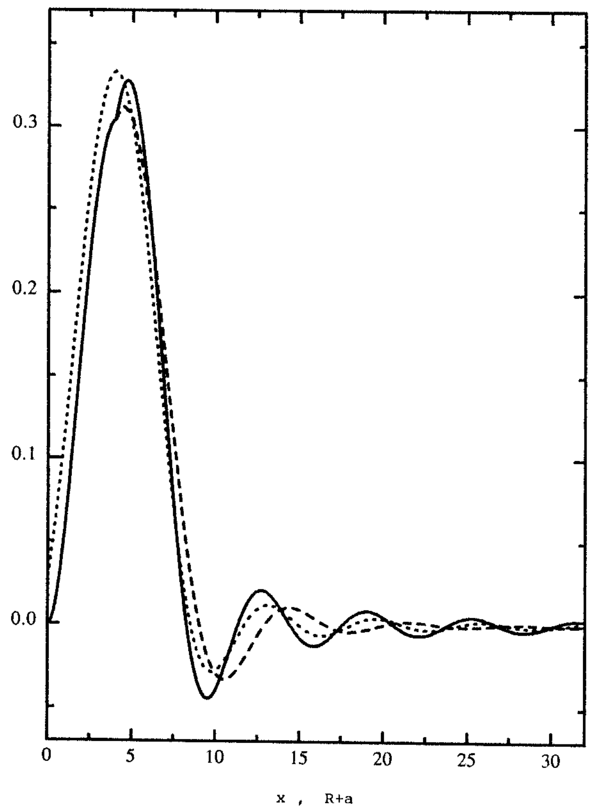

Figure 2

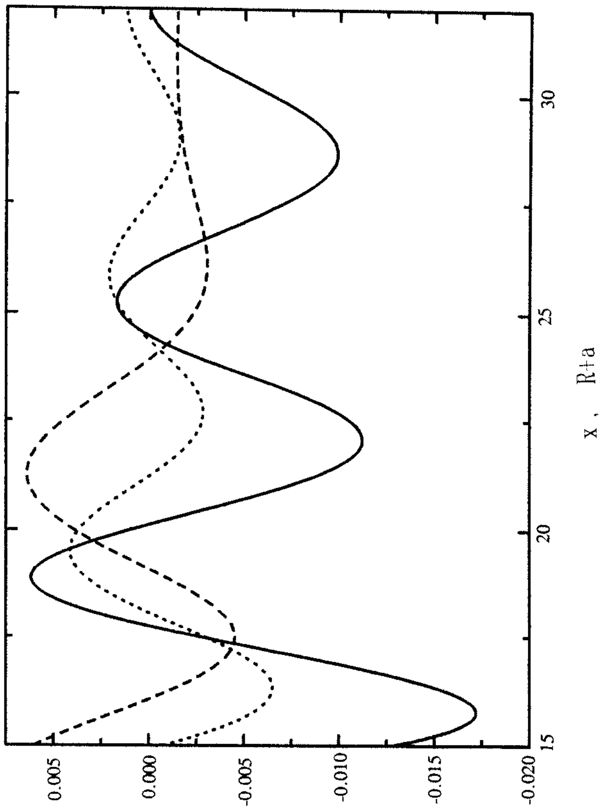

Figure 3

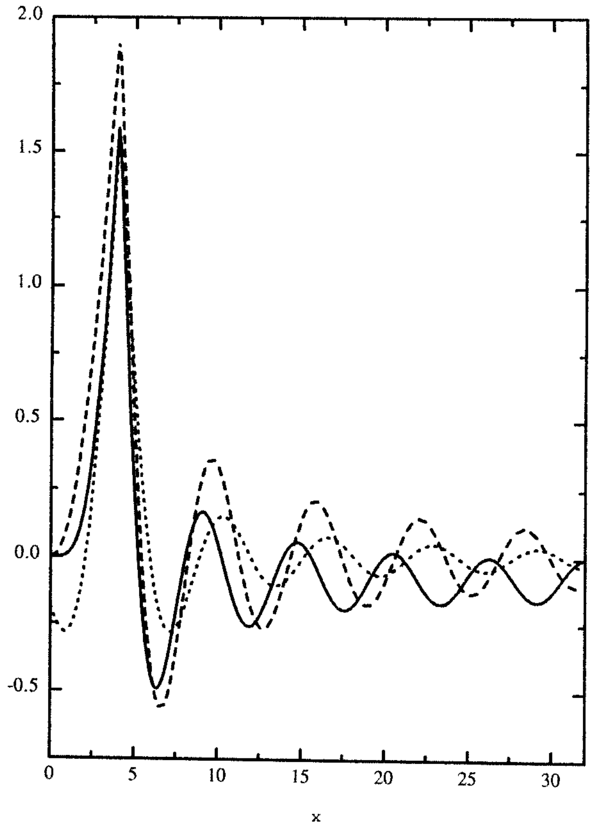

Figure 4

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