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Surface-induced quantum density oscillations in the presence of an external magnetic field

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The electron number density and spin density near the surface of a model metal, semimetal, or semiconductor are calculated in the presence of a uniform magnetic field. The magnetic field is applied in a direction perpendicular to the surface. In this model, the electrons are assumed to be noninteracting and confined between plane parallel surfaces. Numerical results are presented for the limit of a semi-infinite medium. The effect of a magnetic field on the electron density is calculated when the confining potential forming the surface is either an infinite barrier or a finite barrier. The thermal smearing effect of finite temperature is also considered. We conclude that experiments designed to probe the magnetic field dependence of the spin polarization in the surface region would be useful.

I. INTRODUCTION

The effects due to surfaces on the electronic density of a metal, semimetal, or semiconductor, both in the absence and presence of an external magnetic field, continue to receive considerable attention.[1–6] The interesting applications which surface science has found have encouraged both theoretical and experimental investigations leading to the development of techniques which have provided insight into bulk properties as well. We suggest that magnetic fields may be used as probes in providing additional information concerning the effects which a surface has on the electronic properties of metals, semimetals, and semiconductors.

Recently, a calculation of the linear response function $\chi_0(\mathbf{r},\mathbf{r}')$ for a degenerate semi-infinite electron gas in the presence of an external magnetic field perpendicular to the surface was reported.[5] This result provides a means of calculating the effect due to a magnetic field on the electron distribution surrounding an impurity or other static defect embedded in a solid with a surface. In the present study, we discuss two other quantities of interest, i.e., the position-dependent number density $n(\mathbf{r})$ and spin polarization $m(\mathbf{r})$ for a free-electron model with a surface, in the absence of impurities. The surface induces quantum density oscillations (QDO's) in both $n(\mathbf{r})$ and $m(\mathbf{r})$.

In Sec. II the single-particle eigenstates for the electron gas bounded by potential barriers are calculated by solving the Schrödinger equation in the presence of the magnetic field. These solutions are discussed both with the Landau gauge and the radial or circulating gauge for a uniform magnetic field which is applied in the z direction, perpendicular to the surface of the plasma. In the formal development of the present calculation, we allow for the possibility that the potential at the surface forms either a *finite* or *infinite* barrier. The xy dependence of the eigenfunctions is found to be the same as for the bulk system. The sums for the electron number density and spin density are difficult to deal with analytically in the Landau gauge, and we find it convenient to use the wave functions corresponding to the radial gauge. In Sec. III we discuss the infinite-barrier model (IBM). Results for the electron number density for the low-field limit and the high-field quantum limit are derived at zero temperature with this model. These limits have previously been given by Bardeen[6] and by Horing and Yildiz,[2] respectively. We also calculate the explicit temperature dependence for a physically relevant range of values of the temperature and magnetic field strength. Section IV is devoted to a discussion of the finite-barrier model (FBM) at zero temperature. In Sec. V numerical results are presented and discussed.

II. GENERAL FORMULATION OF THE PROBLEM

Consider free electrons in a slab bounded by two parallel planes separated by a distance L and perpendicular to the z axis. Assume periodic boundary conditions in the xy plane parallel to the surface. The boundary conditions are determined by potential barriers at $z=0$ and $z=L$. In this model the confining potential energy $U(z)$ is zero inside the slab and equal to V_0, which can be either finite or infinite, outside the slab.

The electron number density for fixed position $\mathbf{r}$ and spin σ is

$$n_\sigma(\mathbf{r})=\sum_\alpha f_0(E_\alpha^\sigma)\,|\phi_\alpha(\mathbf{r})|^2 . \qquad (2.1\text{a})$$

Here, ϕ_α are wave functions for the stationary states E_α^σ of electrons in a constant magnetic field in the z direction. $f_0(E)=\{1+\exp[\beta(E-\mu)]\}^{-1}$ is the Fermi function, μ is the (magnetic-field-dependent) chemical potential, and $\beta=(k_BT)^{-1}$. With the use of a mathematical identity for the step function in terms of an inverse Laplace transform,[7] Eq. (2.1a) for $n_\sigma(\mathbf{r})$ is given by

$$n_\sigma(\mathbf{r})=-\sum_\alpha \int_0^\infty d\omega \frac{\partial f_0(\omega)}{\partial \omega} \times \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{ds}{2\pi i} \frac{e^{s(\omega-E_\alpha^\sigma)}}{s} |\phi_\alpha(\mathbf{r})|^2 , \tag{2.1b}$$

where γ is a positive constant.

The wave functions ϕ_α are solutions of the Schrödinger equation

$$\left[\frac{1}{2m^*}\left[\frac{\hbar}{i}\nabla+\frac{e}{c}\mathbf{A}\right]^2+U(z)+\frac{g}{2}\sigma\mu_0 H_0\right]\phi_\alpha(\mathbf{r}) = E_\alpha^\sigma \phi_\alpha(\mathbf{r}) . \tag{2.2}$$

Here, $\mathbf{A}$ is the vector potential, $-e$ the charge, and m^* the effective mass of an electron. $\mu_0=e\hbar/2m^*c$ is the spin Bohr magneton and $\sigma=+1$ (-1) for a spin-up (spin-down) electron. All other symbols have their standard meanings. With the use of the Landau gauge $\mathbf{A}=(0,H_0x,0)$, Eq. (2.2) is transformed into the Schrödinger equation of a simple harmonic oscillator, yielding the energy levels explicitly. However, the Landau gauge is inconvenient for calculating $n_\sigma(\mathbf{r})$ in Eq. (2.1) because of the coupling between the x and y quantum numbers.

We have found it convenient to use the radial gauge $\mathbf{A}=\frac{1}{2}H_0\times\mathbf{r}$. Expressing Eq. (2.2) in cylindrical polar coordinates $\mathbf{r}=(\rho,\theta,z)$,

$$-\frac{\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left[\rho\frac{\partial\phi_\alpha}{\partial\rho}\right]+\frac{1}{\rho^2}\frac{\partial^2\phi_0}{\partial\theta^2}+\frac{\partial^2\phi_\alpha}{\partial z^2}\right]+\left[\frac{eH_0}{2m^*c}\frac{\hbar}{i}\frac{\partial}{\partial\theta}+\frac{g}{2}\sigma\mu_0H_0+\frac{e^2H_0^2}{8m^*c^2}\rho^2+U(z)-E_\alpha^\sigma\right]\phi_\alpha=0 . \tag{2.3}$$

The radial, angular, and z dependence of the wave function can be separated by substituting

$$\phi_\alpha(\mathbf{r})=R(\rho)\frac{e^{i\nu\theta}}{\sqrt{2\pi}}\zeta(z) \tag{2.4}$$

into Eq. (2.3), where $\nu=0,\pm1,\pm2,\ldots$, and ζ and R satisfy the equations

$$-\frac{\hbar^2}{2m^*}\frac{d^2\zeta}{dz^2}+\left[U(z)+\frac{\hbar^2k_z^2}{2m^*}\right]\zeta=0 , \tag{2.5a}$$

$$-\frac{\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{d}{d\rho}\left[\rho\frac{dR}{d\rho}\right]-\left[\frac{\nu^2}{\rho^2}+k_z^2\right]R\right]+\left[\frac{e\hbar}{2m^*c}\nu H_0+\frac{g}{2}\sigma\mu_0H_0+\frac{e^2H_0^2}{8m^*c^2}\rho^2-E_\alpha^\sigma\right]R=0 . \tag{2.5b}$$

The values of k_z and the solutions $\zeta\equiv\zeta(z;k_z)$ are determined by the surface boundary conditions. ζ is calculated and applied to the IBM and FBM in Secs. III and IV, respectively.

The solution of Eq. (2.5b) is

$$R(\rho)=\frac{C}{\rho}W_{\kappa,\lambda}(\xi)\equiv\frac{C}{\rho}\xi^{\lambda+1/2}e^{-\xi/2}\Phi(\lambda-\kappa+\tfrac{1}{2};2\lambda+1;\xi) , \tag{2.6}$$

where C is a normalization constant, the Whittaker function $W_{\kappa,\lambda}$ and confluent hypergeometric function Φ are expressed in terms of the variable $\xi\equiv(eH_0/2\hbar c)\rho^2$,

$$\kappa=\frac{1}{2}\left[\frac{1}{\mu_0^*H_0}\left[E_\alpha^\sigma-\frac{\hbar^2k_z^2}{2m^*}\right]-\frac{g}{2}\sigma a-\nu\right] , \tag{2.7a}$$

$$\lambda=\tfrac{1}{2}|\nu| , \tag{2.7b}$$

$a=m^*/m$, and $\mu_0^*=e\hbar/2m^*c$ is the orbital Bohr magneton. We require the solution (2.6) to be regular at $\rho=\infty$ so that $\lambda-\kappa+\frac{1}{2}=-M$, where $M=0,1,2,\ldots$. The stationary-state solutions thus have eigenvalues

$$E_\alpha^\sigma=\frac{\hbar^2k_z^2}{2m^*}+\hbar\omega_c\left[M+\frac{1}{2}+\frac{\nu+|\nu|}{2}+\frac{g}{4}\sigma a\right] , \tag{2.8}$$

where we have introduced the cyclotron frequency $\omega_c\equiv2\mu_0^*H_0/\hbar$. The energy spectrum of Eq. (2.8) is in agreement with the results of the Landau gauge, of course. The normalization constant C is

$$C_{M,|\nu|}=\left[\frac{2\Gamma(M+|\nu|+1)}{M!(\Gamma(|\nu|+1))^2}\right]^{1/2} . \tag{2.9}$$

Substituting Eqs. (2.4) and (2.6)—(2.9) into Eq. (2.1b), we obtain the number density of electrons of spin σ,

$$n_\sigma(\mathbf{r})=-\left[\frac{m^*}{2\pi\hbar^2}\right](\mu_0^*H_0)\int_0^\infty d\omega\frac{\partial f_0(\omega)}{\partial\omega}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{ds}{2\pi i}\frac{1}{s}\exp\left\{s\left[\omega-\frac{\hbar\omega_c}{2}\left[1+\frac{g}{2}\sigma a\right]\right]\right\}$$
$$\times\sum_{k_z}|\zeta(z;k_z)|^2\exp\left[-s\frac{\hbar^2k_z^2}{2m^*}\right]$$
$$\times\sum_{\nu=-\infty}^{\infty}\sum_{M=0}^{\infty}e^{-\xi}C_{M,|\nu|}^2\xi^{|\nu|}\Phi^2(-M;|\nu|+1;\xi)$$
$$\times\exp\left[-s\hbar\omega_c\left[M+\frac{\nu+|\nu|}{2}\right]\right]. \tag{2.10}$$

The ν and M sums are now discussed separately by making use of appropriate generating functions.

We express the confluent hypergeometric function $\Phi(-M;|\nu|+1;\xi)$ in terms of the Laguerre polynomial $L_M^{|\nu|}(\xi)$, and then use Eq. 8.976.1 of Gradshteyn and Ryzhik,[8]

$$\sum_{M=0}^{\infty}C_{M,|\nu|}^2\Phi^2(-M;|\nu|+1;\xi)\exp(-s\hbar\omega_cM)=2\frac{(\xi^2t)^{-|\nu|/2}}{1-t}\exp\left[\frac{2t\xi}{t-1}\right]I_{|\nu|}\left[\frac{2\xi t^{1/2}}{1-t}\right]. \tag{2.11a}$$

For convenience, we have introduced the quantity $t=\exp(-s\hbar\omega_c)$. The ν sum is given by Eq. 8.511.1 of Ref. 8,

$$\sum_{\nu=-\infty}^{\infty}t^{\nu/2}I_{|\nu|}\left[\frac{2\xi t^{1/2}}{1-t}\right]=\exp\left[-\left[\frac{t+1}{t-1}\right]\xi\right]. \tag{2.11b}$$

Substituting Eq. (2.11) into Eq. (2.10), we obtain

$$n_\sigma(\mathbf{r})=n_\sigma(z)=-2\left[\frac{m^*}{2\pi\hbar^2}\right](\mu_0^*H_0)\int_0^\infty d\omega\frac{\partial f_0(\omega)}{\partial\omega}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{ds}{2\pi i}\frac{1}{s}\exp\left\{s\left[\omega-\frac{\hbar\omega_c}{2}\left[1+\frac{g}{2}\sigma a\right]\right]\right\}$$
$$\times\frac{1}{1-\exp(-s\hbar\omega_c)}\sum_{k_z}|\zeta(z;k_z)|^2\exp\left[-\frac{s\hbar^2k_z^2}{2m^*}\right]. \tag{2.12}$$

The result for n_σ in Eq. (2.12) is independent of the spatial coordinates parallel to the surface, as required by translational symmetry along the surface. [It is easily verified that, as a consequence, Eq. (2.12) can be obtained by setting $\xi=0$ in Eq. (2.10) and keeping only the $\nu=0$ contribution to the ν sum.] Further progress in evaluating Eq. (2.12) requires specification of the surface potential and the solution of Eq. (2.5a) in order to evaluate the k_z sum. In the next section we discuss the IBM.

III. INFINITE-BARRIER MODEL

For the infinite-barrier model of a slab of thickness L, the potential energy $U(z)$ is given by $U(z)=0$ for $0<z<L$, and $U(z)=\infty$ for $z<0$ and $z>L$. For this potential, the solution of Eq. (2.5a) is

$$\zeta(z;k_z)=(2/L)^{1/2}\sin(k_zz),\quad k_z=(1,2,3,\ldots)(\pi/L). \tag{3.1}$$

For the *semi-infinite* system ($L=\infty$), we obtain, from Eqs. (2.12) and (3.1),

$$n_\sigma(z)=-2\left[\frac{m^*}{2\pi\hbar^2}\right]^{3/2}(\mu_0^*H_0)\int_0^\infty d\omega\frac{\partial f_0(\omega)}{\partial\omega}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{ds}{2\pi i}\frac{1}{s^{3/2}}\exp\left[s\left[\omega-\frac{g}{2}\sigma a\mu_0^*H_0\right]\right]$$
$$\times\frac{1}{2\sinh(\mu_0^*H_0s)}\left[1-\exp\left[-\frac{2m^*z^2}{\hbar^2s}\right]\right]. \tag{3.2}$$

For illustrative purposes of this model calculation, we set $ag/2\equiv m^*g/2m$ equal to unity. Lifting these restrictions poses no difficulties, but increases the number of parameters.

Making use of standard tables of inverse Laplace transforms,[7] the electron number density $n\equiv n_\downarrow+n_\uparrow$ and the spin polarization taken as $m\equiv(n_\downarrow-n_\uparrow)/n_B$ are given by

$$n(z)=-\frac{4}{\pi^{1/2}}\left[\frac{m^*}{2\pi\hbar^2}\right]^{3/2}(\mu_0^*H_0)\int_0^\infty d\omega\frac{\partial f_0(\omega)}{\partial\omega}\sum_{0\le n<\omega/2\mu_0^*H_0}(2-\delta_{n,0})(\omega-2n\mu_0^*H_0)^{1/2}\times\left\{1-j_0\left[2\left[\frac{2m^*z^2}{\hbar^2}\right]^{1/2}(\omega-2n\mu_0^*H_0)^{1/2}\right]\right\}, \quad (3.3)$$

$$m(z)=-\frac{4}{n_B\pi^{1/2}}\left[\frac{m^*}{2\pi\hbar^2}\right]^{3/2}(\mu_0^*H_0)\int_0^\infty d\omega\frac{\partial f_0(\omega)}{\partial\omega}\omega^{1/2}\left\{1-j_0\left[2\left[\frac{2m^*z}{\hbar^2}\right]^{1/2}\omega^{1/2}\right]\right\}, \quad (3.4)$$

where $j_0(x)\equiv\sin(x)/x$ is a spherical Bessel function and n_B is the electron density in the bulk. We now make use of Eqs. (3.2)—(3.4) to study the electron number density and spin polarization as functions of temperature and magnetic field strength.

A. Zero-temperature regime

In the zero-temperature limit the ω integration in Eqs. (3.3) and (3.4) is trivial. The electron number density and spin polarization are given by the value of the integrand evaluated at $\omega=\mu$. Of course, the chemical potential is dependent on the magnetic field strength. However, the explicit dependence of $m(z)$ on H_0 is only given by the prefactor in Eq. (3.4) as a consequence of setting $ag/2=1$. The dependence of $n(z)$ on magnetic field strength is more involved. We present results for this quantity in two regimes.

The low-magnetic-field limit is easily obtained by expanding the integrand [apart from the factor $\exp(s\omega)$] in Eq. (3.2) in ascending powers of the s variable. This results in an asymptotic expansion in powers of the field strength,

$$n_{\rm LF}(z)=n_0(z)+(\mu_0^*H_0/\mu)^2n_1(z)+\cdots \quad (3.5)$$

(LF denotes low field), where

$$n_0(z)=\frac{k_F^3}{3\pi^2}\left[1+3\left[\frac{\cos(2k_Fz)}{(2k_Fz)^2}-\frac{\sin(2k_Fz)}{(2k_Fz)^3}\right]\right], \quad (3.6)$$

$$n_1(z)=\frac{k_F^3}{3\pi^2}[1-\cos(2k_Fz)] . \quad (3.7)$$

We emphasize that the asymptotic expansion has isolated only the *explicit* magnetic field dependence. There is additional magnetic field dependence due to the fact that the chemical potential $\mu=\mu(H_0)$ is field dependent. That is, the requirement that $n(z)$ in Eq. (3.5) reproduces exactly for $z\rightarrow\infty$ the known zero-field electron density, $n_B=k_F^3(0)/3\pi^2$, implies

$$\mu(H_0)/\epsilon_F=1-\tfrac{1}{6}(\mu_0^*H_0/\epsilon_F)^2+O(H_0^4) , \quad (3.8)$$

where $\epsilon_F\equiv\mu(0)$ is the Fermi energy. The wave number k_F in Eqs. (3.6) and (3.7) depends on the magnetic field, with

$$k_F=k_F(H_0)\equiv(2m^*\mu(H_0)/\hbar^2)^{1/2} .$$

In the absence of a magnetic field, $n_0(z)$ in Eq. (3.6) is exactly Bardeen's result.[6]

In the high-field quantum limit (HFQL), $\mu_0^*H_0\gg\mu$. In this limit, the value of $n(z)$ can be obtained by expanding the s integral in Eq. (3.2) around $s=\infty$. Each term in this expansion correpsonds to the inclusion of one more Landau level. The result when only the leading term is retained,

$$n_{\rm HFQL}(z)=(m^*\mu_0^*H_0/\pi^2\hbar^2)k_F\left[1-\frac{\sin(2k_Fz)}{2k_Fz}\right], \quad (3.9)$$

was first calculated by Horing and Yildiz.[2] Further discussion of the magnetic-field-dependent $n(z)$ has not previously been given. Equation (3.9) corresponds exactly to the $n=0$ term in Eq. (3.3), evaluated at zero temperature.

In the limit as $z\rightarrow\infty$, we must have $n_{\rm LF}=n_{\rm HFQL}$ so that, from Eqs. (3.6) and (3.9),

$$k_F(H_0)=\tfrac{2}{3}k_F^3(0)r_0^2 \quad (3.10)$$

in the high-field regime, where r_0 is the cyclotron radius defined by $r_0^{-2}\equiv eH_0/\hbar c$. Therefore, *near* the surface we have

$$n_{\rm HFQL}/n_{\rm LF}\approx\tfrac{20}{27}[k_F(0)r_0]^4 . \quad (3.11)$$

This means that the electron number density is reduced near the surface in the presence of a high magnetic field (also see Sec. V).

B. Effect of temperature on the QDO

Integrating Eq. (3.3) by parts in a straightforward way, we obtain

$$n(z)=\frac{2}{\pi^{1/2}}\left[\frac{m^*}{2\pi\hbar^2}\right]^{3/2}(\mu_0^* H_0)\int_0^\infty d\omega\, f_0(\omega)\sum_{0\le n<\omega/2\mu_0^* H_0}(2-\delta_{n,0})(\omega-2n\mu_0^* H_0)^{-1/2}\times\left\{1-\cos\left[2\left[\frac{2m^* z^2}{\hbar^2}\right]^{1/2}(\omega-2n\mu_0^* H_0)^{1/2}\right]\right\}. \tag{3.12}$$

We now discuss the damping of the QDO in the high-field quantum limit, and at sufficiently low temperature when $k_B T \ll \mu \ll \hbar\omega_c$. In this limit, with $n(z)\equiv n_B+\delta n(z)$, we have

$$\delta n(z)=-\left[\frac{m^*}{2\pi^2\hbar^2}\right](\mu_0^* H_0)\int_0^\infty dk\, f_0(\epsilon_k)\cos(2kz)\,, \tag{3.13a}$$

where $\epsilon_k\equiv\hbar^2 k^2/2m^*$. Equation (3.13a) can be evaluated by a contour integration.[9] For any fixed, large value of z, and at low temperatures, it is sufficient to approximate the poles, in the upper half k plane, of the Fermi function, by $\pm k_F+(2n+1)\pi i k_F/2\beta\mu$, where $n=0,1,2,\ldots$. This leads to the usual thermal damping factor $\sinh(\pi k_F z/\beta\mu)$, and results in

$$\delta n(z)\approx-\left[\frac{m^*}{2\pi\hbar^2}\right](\mu_0^* H_0)\frac{k_F}{2\beta\mu}\sin(2k_F z)\Big/\sinh\left[\frac{\pi k_F z}{\beta\mu}\right]. \tag{3.13b}$$

Note that the $T=0$ limit of Eq. (3.13b) reproduces exactly the oscillatory part of Eq. (3.9), as should be expected, for all z. When both z and T are small and $\pi k_F z/\beta\mu$ is not small, the temperature dependence of $n(z)$ can be described by the usual small Sommerfeld corrections.

The exact result in Eq. (3.3) for the electron number density in the presence of a magnetic field should be compared with the corresponding result in the absence of a magnetic field, at arbitrary temperature. Substituting

$$\phi(\mathbf{r})=\exp(i\mathbf{k}_{\|}\cdot\rho)\sin(k_z z)/(2\pi^3)^{1/2}$$

into Eq. (2.1b), we obtain

$$n(z)=-2\left[\frac{m^*}{2\pi\hbar^2}\right]^{3/2}\int_0^\infty d\omega\frac{\partial f_0(\omega)}{\partial\omega}\omega^{3/2}\times\left[\frac{1}{\Gamma(\frac{5}{2})}-\frac{J_{3/2}(2k_\omega z)}{(k_\omega z)^{3/2}}\right], \tag{3.14}$$

where $k_\omega\equiv(2m^*\omega/\hbar^2)^{1/2}$, and $J_{3/2}$ is a Bessel function of the first kind. Just as for Eq. (3.13b), it can be shown that, for $\beta\mu\gg1$ and large fixed z, the QDO's of $n(z)$ in Eq. (3.14) are also damped exponentially. Of course, this thermal damping also applies to the spin polarization.

IV. FINITE-BARRIER MODEL

In this section we calculate the electron-spin density $n_\sigma(z)$ for the finite-barrier model. For this calculation we need the energy eigenvalues and wave functions for an electron confined by the potential barrier

$$U(z)=\begin{cases}V_0 & \text{for } z<0 \text{ and } z>L\,,\\ 0 & \text{for } 0<z<L\,.\end{cases} \tag{4.1}$$

For simplicity, we first consider zero temperature. This means that we only need the class of eigenstates with energies less than the barrier height V_0. Of these, only energies less than the chemical potential will be required.

Since the potential barrier is symmetric about its midplane at $z=L/2$, the solutions of Eq. (2.5a) have either even or odd parity with respect to the variable z. Let

$$k_z^2=k_0^2-\kappa^2,\quad k_0^2\equiv 2m^* V_0/\hbar^2\,. \tag{4.2}$$

The symmetric (S) and antisymmetric (A) solutions of Eq. (2.5a) are given by[10]

$$\zeta_S(z)=\begin{cases}N_S\cos\left[k_z\left[z-\frac{L}{2}\right]\right], & 0\le z-L/2\le L/2\\ N_S\cos\left[k_z\frac{L}{2}\right]e^{\kappa(L-z)}, & z\ge L\end{cases} \tag{4.3a}$$

$$\zeta_S(L/2-z)=\zeta_S(z-L/2)\,, \tag{4.3b}$$

$$\frac{1}{N_S^2}=\frac{1}{k_z}\left[k_z\frac{L}{2}+\sin\left[k_z\frac{L}{2}\right]\cos\left[k_z\frac{L}{2}\right]\right]+\frac{1}{\kappa}\cos^2\left[k_z\frac{L}{2}\right], \tag{4.3c}$$

and

$$\zeta_A(z)=\begin{cases}N_A\sin\left[k_z\left[z-\frac{L}{2}\right]\right], & 0\le z-L/2\le L/2\\ N_A\sin\left[k_z\frac{L}{2}\right]e^{\kappa(L-z)}, & z\ge L\end{cases} \tag{4.4a}$$

$$\zeta_A(L/2-z)=-\zeta_A(z-L/2)\,, \tag{4.4b}$$

$$\frac{1}{N_A^2}=\frac{1}{k_z}\left[k_z\frac{L}{2}-\sin\left[k_z\frac{L}{2}\right]\cos\left[k_z\frac{L}{2}\right]\right]+\frac{1}{\kappa}\sin^2\left[k_z\frac{L}{2}\right] . \tag{4.4c}$$

The amplitudes inside and outside of the potential barrier have been adjusted so that ζ is continuous at $z=L$. $N_{S,A}$ are normalization constants. Continuity of $d\zeta/dz$ at $z=L$ then quantizes the k_z values. These are given by

$$\tan\left[k_z\frac{L}{2}\right]=\frac{\kappa}{k_z}\quad (S\text{ solutions}) , \tag{4.5a}$$

$$\tan\left[k_z\frac{L}{2}\right]=-\frac{k_z}{\kappa}\quad (A\text{ solutions}) . \tag{4.5b}$$

With the use of Eqs. (4.5) in Eqs. (4.3c) and (4.4c), we obtain

$$N_{S,A}^2=L/2+1/\kappa . \tag{4.6}$$

Taking the limit $L\to\infty$ for a semi-infinite medium, we may write both the even- and odd-parity states as

$$\zeta(z)=\begin{cases}(2/\pi)^{1/2}\sin(k_z z+\delta), & z\geq 0\\ (2/\pi)^{1/2}\sin(\delta)e^{\kappa z} , & z\leq 0\end{cases} \tag{4.7}$$

where $\tan\delta=k_z/\kappa$. Substituting Eq. (4.7) into Eq. (2.12), we obtain the electron-spin density for the FBM at zero temperature. For $z\geq 0$, we have

$$n_\sigma(z)=\frac{4}{\pi}\left[\frac{m^*}{2\pi\hbar^2}\right](\mu_0^*H_0)\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{ds}{2\pi i}\frac{1}{s}\frac{1}{2\sinh(\mu_0^*H_0 s)}\times\int_0^{k_0}dk_z\exp\left[\frac{s\hbar^2}{2m^*}(k_\sigma^2-k_z^2)\right]\left[\sin^2(k_z z)+\frac{k_z^2}{k_0^2}\cos(2k_z z)+\frac{k_z(k_0^2-k_z^2)^{1/2}}{k_0^2}\sin(2k_z z)\right], \tag{4.8}$$

where $k_\sigma\equiv[2m^*(\mu-\mu_0^*H_0\sigma)/\hbar^2]^{1/2}$. For $z<0$ we have

$$n_\sigma(z)=\frac{4}{\pi}\left[\frac{m^*}{2\pi\hbar^2}\right](\mu_0^*H_0)\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{ds}{2\pi i}\frac{1}{s}\frac{1}{2\sinh(\mu_0^*H_0 s)}\int_0^{k_0}dk_z\exp\left[\frac{s\hbar^2}{2m^*}(k_\sigma^2-k_z^2)\right]\frac{k_z^2}{k_0^2}e^{2\kappa z} . \tag{4.9}$$

The inverse Laplace transform in Eqs. (4.8) and (4.9) may be calculated with the use of standard tables.[7] We obtain

$$\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{ds}{2\pi i}\frac{1}{s}\frac{1}{2\sinh(\mu_0^*H_0 s)}\exp\left[\frac{s\hbar^2}{2m^*}(k_\sigma^2-k_z^2)\right]=\sum_{n=0}^{\infty}\Theta\left[k_\sigma^2-k_z^2-\frac{2m^*}{\hbar}(n+\tfrac{1}{2})\omega_c\right] . \tag{4.10}$$

The upper limit on the k_z integrals of Eqs. (4.8) and (4.9) is thus correctly reduced to $[k_\sigma^2-2m^*(n+\frac{1}{2})\omega_c/\hbar]^{1/2}$, as is appropriate at zero temperature. Taking the limit $H_0\to 0$ in Eqs. (4.8) and (4.9), we obtain Stratton's result[4] for the electron number density for the FBM in the absence of a magnetic field.

At finite temperature, electron states of energy larger than the chemical potential will contribute. The highly excited states (including those with energy eigenvalues $E>V_0$) give exponentially small contributions to the electron density at low temperatures, and thus can be neglected for present purposes. There will, of course, be thermal smearing (as in the preceding section) of the QDO at large distances from the surface.

V. NUMERICAL RESULTS

In this section we present numerical results for the electron number density and spin polarization for both the IBM and FBM. We first note that since the electron number density tends toward its bulk value n_B well *inside* the medium, the chemical potential must satisfy

$$n_B=-2\left[\frac{m^*}{2\pi\hbar^2}\right]^{3/2}(\mu_0^*H_0)\int_0^\infty d\omega\frac{\partial f_0(\omega)}{\partial\omega}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{ds}{2\pi i}\frac{e^{s\omega}}{s^{3/2}}\frac{\cosh(\frac{1}{2}g\mu_0H_0 s)}{\sinh(\mu_0^*H_0 s)} . \tag{5.1}$$

At zero temperature, Eq. (5.1) agrees with Eq. (3.8) of Ref. 11. When the electron g factor and electron effective mass are chosen such that $m^*g/2m=1$ for the degenerate electron gas, Eq. (5.1) becomes

$$n_B=\frac{4}{\pi^{1/2}}\left[\frac{m^*}{2\pi\hbar^2}\right]^{3/2}(\mu_0^*H_0)\sum_{0\leq n<\mu/2\mu_0^*H_0}(2-\delta_{n,0})(\mu-2n\mu_0^*H_0)^{1/2} . \tag{5.2}$$

In the high-field quantum limit, when only the lowest Landau level is occupied, the $n=0$ term in Eq. (5.2) gives the chemical potential[11]

$$\mu/\varepsilon_F = \tfrac{4}{9}(\varepsilon_F/\mu_0^* H_0)^2 \, . \tag{5.3}$$

The purpose of the numerical calculations is to display the characteristics of the electron density of a semi-infinite degenerate plasma in the presence of a uniform magnetic field. The calculations for $n(z)$ are based on Eq. (3.3) at $T=0$ for the IBM and Eqs. (4.8)–(4.10) for the FBM.

Numerical results for the electron number density of the degenerate, semi-infinite jellium model are presented in Figs. 1 and 2. The electron number density in the bulk plasma is chosen as $n_B = 10^{17}$ cm^{-3}. The orbital effective mass of an electron is chosen as $m^* = 0.01m$. In the absence of a magnetic field, the Fermi energy $\epsilon_F \approx 0.1$ eV and the Fermi wave number $k_F(0) \approx 0.01$ Å^{-1}. For the FBM the surface potential barrier is set equal to $V_0 = 2\epsilon_F$. For a magnetic field of strength $H_0 = 50$ kG, only the *two* lowest Landau levels are occupied. When the magnetic field is increased to $H_0 = 150$ kG, the high-field quantum-limit condition is achieved and the electrons occupy the lowest Landau level *only*.

We have plotted $n(z)$ in Fig. 1 for the IBM and in Fig. 2 for the FBM, as a function of z for various field strengths. The general features are similar for the IBM and FBM, except for the fact that $n(z)$ vanishes at the surface $z=0$ for the IBM, but decays exponentially in the region $z<0$ for the FBM. Note that for z in the surface region [taken as $|z| \lesssim k_F^{-1}(0)$], $n(z)$ is reduced in the high-field quantum limit relative to its value in the absence of a magnetic field, as expected in Sec. III. The

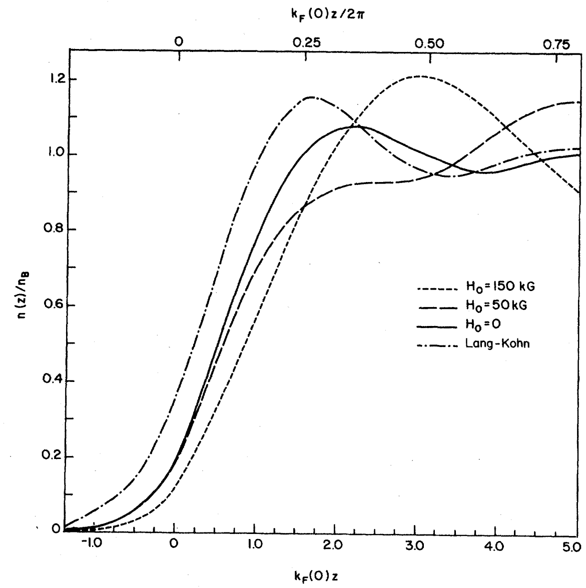

FIG. 2. Same as Fig. 1, except that the surface potential barrier is finite. The self-consistently calculated density of Lang and Kohn (Ref. 13) for $r_s = 6$ is also shown in order to indicate the modifications due to proper treatment of Coulomb interactions. Details are given in the text.

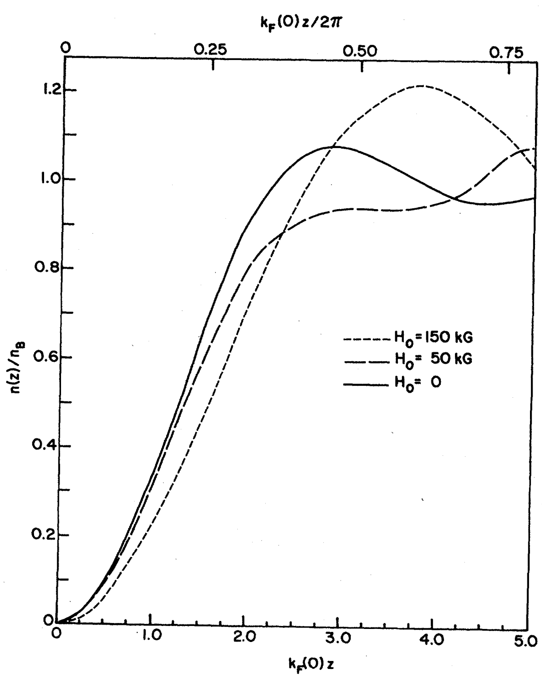

FIG. 1. Total number density for free electrons confined by an infinite potential barrier to the semi-infinite domain $z>0$. The curves are plotted as a function of the distance z from the surface. The solid line is for zero magnetic field strength. The two other curves illustrate the effects due to a magnetic field. n_B is the electron number density in the bulk plasma. $2\pi/k_F(0)$ is the Fermi wavelength in the absence of a magnetic field.

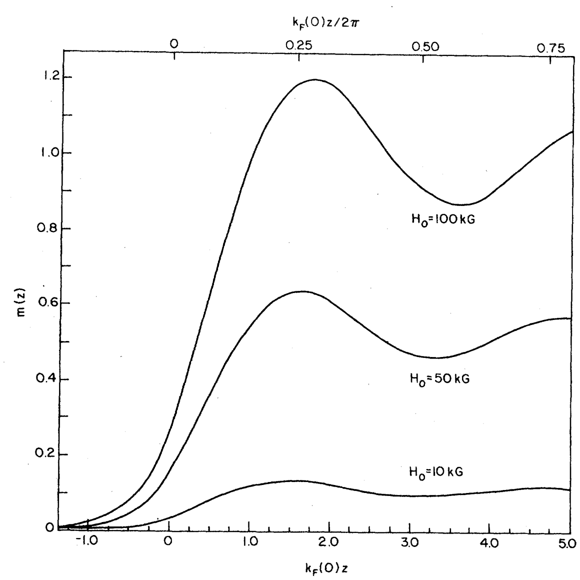

FIG. 3. Spin polarization $m(z)$ for the finite-barrier model. Details are given in the text.

electron number density increases as z increases and reaches the bulk value far inside the sample in the usual oscillatory way. The effect of the magnetic field on the amplitude of the QDO is significant ($\sim 30\%$) in the region where $z \sim k_F^{-1}(0)$. In Fig. 3 we have plotted the spin polarization, defined as

$$m(z) = [n_\downarrow(z) - n_\uparrow(z)]/n_B$$

for magnetic fields $H = 10$, 50, and 100 kG as a function of z for the FBM (again with $V_0 = 2\epsilon_F$). Results for the IBM are very similar. Note that $n(z)$ and $m(z)$ for both the IBM and the FBM correctly reproduce the bulk number density and spin density, respectively, for $z \rightarrow \infty$.

We are now in a position to draw some conclusions. From the above results we see that the particle density and spin polarization are not extremely sensitive to V_0/ϵ_F, at least for the relevant range of parameters considered here. We find that the effect of the applied magnetic field on surface-induced QDO's can be as substantial as the magnetic field effects on QDO's induced by static impurities near surfaces.[12] Finally, the spin polarization has been found to be extremely sensitive to the applied magnetic field, for both the IBM and FBM, except in the high-field quantum limit, where the spin density essentially saturates. This suggests that experiments designed to probe the magnetic field dependence of the spin polarization in the surface region would be very informative.

We emphasize that the aim of the present work has been to examine the degree of sensitivity to an applied magnetic field of the electron number density and spin polarization for a plasma with a planar surface. As a first step, the simplest model for noninteracting electrons was used to obtain some numerical results, and the effect of Coulomb interactions has been neglected. We expect on general grounds that these affect the phase and, to a lesser extent, the amplitude of the oscillations for $n(z)$ and $m(z)$. Unfortunately, we know of no calculations for the electron number density in a bounded plasma with electron-electron interactions in the presence of an external magnetic field. This is a very nontrivial problem. However, there are results for $n(z)$ in the absence of an external magnetic field which have been obtained self-consistently by Lang and Kohn,[13] and which are illustrated in Fig. 2 for $r_s = 6$, the lowest density reported there. It is seen that in the presence of Coulomb interactions the amplitude of the oscillations is roughly the same as for noninteracting electrons, but the phase of these oscillations is shifted, as expected. It is expected that in the presence of an external magnetic field the results for $n(z)$ would show comparable sensitivity to electron-electron interactions. Regarding the spin polarization, we are not aware of any calculations for an interacting bounded plasma, except in the very-weak-magnetic-field limit. Again, on quite general grounds, we expect that the phase and amplitude of the QDO's in $m(z)$ will be somewhat sensitive to the details, including the electron-electron interactions in some appropriate approximation. However, the extreme sensitivity of $m(z)$ to the strength of the applied magnetic field will persist. Consequently, the present model of noninteracting electrons should provide a useful initial indication of the sensitivity of charge and spin densities to applied magnetic fields.

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