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Multiple-boundary-reflection effects on Friedel oscillatory phenomena in a quantising magnetic field

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Abstract. We examine the effects on Friedel oscillations of multiple boundary reflections of electron wavefunctions confined to a plasma slab. The bounding surface is simulated by two infinite-barrier planar boundaries in the presence of a normal quantising magnetic field. To exhibit such Friedel oscillatory features in the presence of multiple boundary reflections, we determine the free-electron density perturbation response function of a finite slab of degenerate Landau quantised plasma in a real-space representation explicitly. In this we employ an appropriate superposition of infinite-space-image Green functions to impose the boundary condition of specular reflection of electrons at the slab faces. The magnetic field is applied perpendicular to the boundary planes. Our real-space results for the static limit of the free-electron density perturbation response function in a magnetic field are evaluated in the quantum strong-field limit, as well as in low/intermediate magnetic fields, and de Haas–van Alphen oscillatory terms are also exhibited. Manifestations of the role of multiple boundary reflections in Friedel oscillatory phenomena are clearly evident in these results.

1. Introduction

Friedel oscillatory screening phenomena have long been the focus of considerable interest in degenerate solid state plasmas, both in the absence and presence of an external magnetic field [1]. Moreover, the introduction of a boundary generates a perturbation which induces a Friedel oscillatory density/potential response of the quantum plasma, particularly in the direction parallel to a quantising magnetic field normal to the planar surface. The time-independent static limit of such a response for a semi-infinite quantum plasma has been examined for arbitrary magnetic field strength by Glasser, Geldart and Gumbs [2], and for null magnetic field by Rudnick [3]. We shall examine the effects on Friedel oscillations of multiple boundary reflections of electron wavefunctions confined to a plasma slab by two infinite-barrier planar bounding surfaces in a normal quantising magnetic field. To exhibit such Friedel oscillatory features in the presence of multiple boundary reflections, we determine the free electron density perturbation response of a finite slab of degenerate Landau quantised plasma in a real space representation explicitly. To facilitate this analysis we employ a superposition of properly positioned infinite-space image Green's functions to impose the boundary condition of specular

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reflection of electrons at the slab faces. In this, we focus attention on the nonlocal density perturbation response function $R(1,2) = \delta\rho(1)/\delta V(2)$ where $\rho(1)$ is the perturbed density at space time point $1 = \boldsymbol{r}_1, \boldsymbol{t}_1$ generated by the effective potential $V(2)$. Alternatively expressed,

$$\rho(1) = \int \mathrm{d}^4(1')\, R(11')V(1')$$

and it is immediately evident that the model potential $V(1') = \delta^{(3)}(\boldsymbol{r}_1' - \boldsymbol{r}_2)\mathrm{e}^{-\mathrm{i}\Omega t_1'}$ induces the density perturbation as $R(\boldsymbol{r}_1, \boldsymbol{r}_2; \Omega)$ at the driving frequency (that is, $\rho(1) = R(\boldsymbol{r}_1, \boldsymbol{r}_2; \Omega)\mathrm{e}^{-\mathrm{i}\Omega t_1}$), so R is appropriate as a vehicle for the description of Friedel oscillatory phenomenon in density response subject to multiple boundary reflections in a magnetic field. In this analysis of the density response, we employ the free electron ring diagram $R(1,2) = -\bar{G}(12)\bar{G}(21^+)$, where $\bar{G}(12)$ is the equilibrium one-electron thermodynamic Green's function in the absence of interparticle interactions, and for the finite slab $z = 0 \rightarrow d$ the boundary condition of specular reflection must be imposed such that $\bar{G}(12)$ vanishes for $z_1 = 0, d$ and $z_2 = 0, d$. The resulting time-dependent free electron slab density perturbation response function $R(12)$ in magnetic field was first reported in a momentum space representation by Horing and Yildiz [1]. In order to gain an appreciation of the effects of multiple boundary reflections on Friedel oscillatory phenomena we shall determine $\rho(1) \sim R(\boldsymbol{r}_1, \boldsymbol{r}_2)$ in a real space representation explicitly. The appropriate Green's function for electrons subject to the boundary condition of specular reflection at the slab faces has been expressed as a superposition of infinite space Green's functions $\bar{G}_\infty(1,2)$ in the literature [4], and it has the property of vanishing at the slab faces along with the electron wavefunctions:

$$\bar{G}(r_1 t_1, r_2 t_2) = \sum_{n=-\infty}^{\infty} [\bar{G}_\infty(\bar{R}, z_1, 2nd + z_2; T) - \bar{G}_\infty(\bar{R}, z_1, 2nd - z_2; T)] \tag{1}$$

where $T = t_1 - t_2$ and $\bar{R} = \bar{r} - \bar{r}_2 = (x_1 - x_2, y_1 - y_2)$. $R(12)$ may be written in frequency Ω representation as

$$R(r_1, r_2; \Omega) = 1\left(\int_0^\infty \mathrm{d}T\, \mathrm{e}^{-\mathrm{i}(\Omega - \mathrm{i}\delta)T} \bar{G}^{>}(r_1, r_2; T)\bar{G}^{<}(r_2 m\, r_1 l - T)\right)^*$$
$$+ -\mathrm{i}\int_{-\infty}^0 \mathrm{d}T\, \mathrm{e}^{-\mathrm{i}(\Omega + \mathrm{i}\delta)T} \bar{G}^{<}(r_1, r_2; T)\bar{G}^{>}(r_2, r_1; -T) \tag{2}$$

where $G^{\gtrless}$ is given in terms of $\bar{G}_\infty^{\gtrless}$ as in (1), and the magnetic-field-dependent infinite-space thermodynamic Green function $G_\infty^{\gtrless}$ is obtained as [5] ($\hbar = 1$)

$$\bar{G}_\infty^{\gtrless}(r_1, r_2; T) = \mathrm{e}^{\mathrm{i}\zeta T} C(r_1, r_2) \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \begin{pmatrix} \mathrm{i}(f_0(\omega) - 1) \\ \mathrm{i}f_0(\omega) \end{pmatrix} \mathrm{e}^{\mathrm{i}\omega T}$$
$$\times \int_{-\infty}^{\infty} \mathrm{d}T'\, \mathrm{e}^{\mathrm{i}\omega T'} \frac{1}{(2\pi^{1/2})^3} \left(\frac{2m^*}{\mathrm{i}T'}\right)^{1/2} \times \frac{m^*\omega_c}{\mathrm{i}\sin(\omega_c T'/2)} \mathrm{e}^{-\mathrm{i}\mu_0 H \sigma_3 T'}$$
$$\times \exp[\tfrac{1}{4}\,\mathrm{I}m^*\omega_c \bar{R}^2 \cot(\omega_c T'/2)] \exp\left(\frac{\mathrm{i}m^*}{2T'}(z_1 - z_2)^2\right). \tag{3}$$

The notation of [5] is generally maintained here. (ζ = chemical potential = Fermi energy for zero temperature, $f_0(\omega)$ = Fermi–Dirac distribution function, μ_0, μ_0^* = spin, orbital Bohr magneton, H = magnetic field, σ_3 = Pauli spin matrix No 3, m^* = effective mass of the electron, ω_c = cyclotron frequency eH/m^*c.) Also

$$C(r_1, r_2) \equiv \exp[\mathrm{i}(\tfrac{1}{2}e r_1 \cdot \boldsymbol{H} \times r_2 - \varphi(r_1) + \varphi(r_2))]$$

for arbitrary gauge function $\varphi(r)$.

After some straightforward but lengthy manipulations, the result of (2) for $R(r_1, r_2; \Omega)$ at zero temperature may be obtained using (3) as follows:

$$R(r_1,r_2;\Omega) = -2(\mu_0^* H)^2(m^*/2\pi)^3 \int_{-\mathrm{i}\infty+\delta}^{\mathrm{i}\infty+\delta} \frac{\mathrm{d}s}{2\pi\mathrm{i}} \mathrm{e}^{s\xi}\biggl(s^{-1}\int_0^1 \frac{\mathrm{d}u}{\sqrt{uu'}} \frac{\cosh(\alpha s)}{\sinh(su)\sinh(su')}$$

$$\times \exp[-\frac{su'}{\mu_\delta^* H}(\Omega + \mathrm{i}\delta)] \exp\{-a[\coth(su) + \coth(su')]\bar{R}^2]$$

$$\times \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} \{\exp[-a(z_1 - 2nd - z_2)^2/su] - \exp[-a(z_1 - 2nd + z_2)^2/su]\}$$

$$\times \{\exp[-a(z_1 - 2md - z_2)^2/su'] - \exp[-a(z_1 - 2md + z_2)^2/su']\}\biggr) \qquad (4)$$

where the s-integration is performed over the standard inverse Laplace transform contour; $u' = 1 - u$; $\xi = \zeta/\mu_0^* H$; α is the effective mass in units of the electron mass and $a = m^* \mu_0^* H/2$. In this study of Friedel oscillatory phenomena with multiple boundary reflections in various regimes of magnetic field strength, we examine the static limit of (4), $\Omega \to 0$, henceforth. Here, we distinguish two classes of terms in the density perturbation response function on the basis of their roles in the associated electrostatic polarisability of the finite slab plasma. Those terms which correspond to the plasma having bulk polarisation properties uniformly throughout the slab, subject to electrostatic joining conditions [6] across the slab boundaries on either side [7–12], are termed 'classical' and bear the subscript 'cl'. It should be noted that this is somewhat of a misnomer since the bulk properties presumed to uniformly permeate the slab in this class of terms do in general involve infinite space quantum effects. Other quantum effects associated with the vanishing of wavefunctions, Green's functions and density at the slab boundaries (by which the boundaries induce spatially inhomogeneous modifications of the polarisability in the slab, so that it is not in fact uniform throughout the slab), are excluded from the 'classical' terms, and the remaining terms involving such effects are termed 'quantum interference' terms [13–14], bearing the subscript 'QI'. In total, $R = R_{\mathrm{cl}} + R_{\mathrm{QI}}$.

2. Low magnetic field strength

For low magnetic fields, $\xi \gg 1$, we develop the monotonic dependence of $R(r_1, r_2; \Omega = 0)$ in a series of inverse powers of ξ; $R = R(0) + (R^{(1a)} + R^{(1b)})\xi^{-2} + \dots$ The execution of the s- and u-integrals (using the integrals tabulated in the Appendix, and noting the $u \leftrightarrow u'$ symmetry) leads to results for the 'classical (cl) and 'quantum interference' (QI) parts as follows:

$$r_1(n) \equiv (x_1, y_1, z_1 + 2nd) = (x_1, y_1, z_1(n)) \qquad r_1'(n) \equiv (x_1, y_1, -z_1(n))$$

$$R_{1,2_n} = r_1 - r_2(n) \qquad R_{1,2_n'} = r_1 - r_2'(n)$$

$$z_{1,2_n} = z_1 - z_2(n) \qquad z_{1,2'_n} = z_1 + z_2(n)$$

$$R^{(0)}_{\mathrm{cl}}(r_1, r_2; \Omega = 0) = -\frac{m^* k_{\mathrm{F}}^2}{2\pi^3} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} [(R_{1,2_n} R_{1,2_m})^{-1} j_1(k_{\mathrm{F}}(R_{1,2_n} + R_{1,2_m})) + (R_{1,2'_n} R_{1,l_m})^{-1} j_1(k_{\mathrm{F}}(R_{1,2'_n} + R_{1,2'_m}))] \tag{5a}$$

$$R^{(0)}_{\mathrm{QI}}(r_1, r_2; \Omega = 0) = \frac{m^* k_{\mathrm{F}}^2}{\pi^3} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} (R_{1,2'_n} R_{1,2_m})^{-1} j_1(k_{\mathrm{F}}(R_{1,2'_n} + R_{1,2_m})) \tag{5b}$$

$$R^{(1a)}_{\mathrm{cl}}(r_1 r_2; \Omega = 0) = \frac{m^* k_{\mathrm{F}}^4}{48\pi^3} \bar{R}^2 \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left(\frac{\sin(k_{\mathrm{F}}(R_{1,2_n} + R_{1,2_m}))}{R_{1,2_n} R_{1,2_m}} + \frac{\sin(k_{\mathrm{F}} R_{1,2'_n} + R_{1,2'_m}))}{R_{1,2'_n} R_{1,2'_m}} \right) \tag{6a}$$

$$R^{(1a)}_{\mathrm{QI}}(r_1, r_2; \Omega = 0) = -\frac{m^* k_{\mathrm{F}}^4}{24\pi^3} \bar{R}^2 \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} (\bar{R}_{1,2'_n} R_{1,2_m})^{-1} \times \sin(k_{\mathrm{F}} R_{1,2'_n} + R_{1,2_m})) \tag{6b}$$

$$R^{(1b)}_{\mathrm{cl}}(r_1, r_2; \Omega = 0) = -\frac{m^* k_{\mathrm{F}}^4}{16\pi^3} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left[\alpha^2 \left(\frac{R^{+}_{1,2_n} R_{1,2_m})}{k_F R_{1,2_n} R_{1,2_m}} \cos(k_{\mathrm{F}}(R_{1,2_n} + R_{1,2_m})) + \frac{(R_{1,2'_n} R_{1,2'_m})}{k_{\mathrm{F}} R_{1,2'_n} R_{1,2'_m}} \cos(k_{\mathrm{F}}(R_{1,2'_n} + R_{1,2'_m})) - \tfrac{1}{3}[\Psi_0(k_{\mathrm{F}} R_{1,2_m}, k_{\mathrm{F}} R_{1,2_n}) + \Psi_0(k_{\mathrm{F}} R_{1,2'_m}, k_{\mathrm{F}} R_{1,2'_n})] \right] \tag{6c}$$

$$R^{(1b)}_{\mathrm{QI}}(r_1, r_2; \Omega = 0) = \frac{m^* k_{\mathrm{F}}^4}{8\pi^3} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left[(\alpha^2 - \tfrac{1}{3}) \times \left(\frac{R_{1,2_n} + R_{1,2'_m}}{k_{\mathrm{F}} R_{1,2_n} R_{1,2'_m}} \right) \cos(k_{\mathrm{F}}(R_{1,2_n} + R_{1,2'_m})) - \tfrac{2}{3} \mathrm{Si}\left(\frac{k_{\mathrm{F}}}{2} (R_{1,2_n} + R_{1,2'_m}) \right) \right]. \tag{6d}$$

Here $k_{\mathrm{F}} = (2m^* \zeta)^{1/2}$ also has magnetic field dependence, $\mathrm{Si}(x)$ denotes the sine integral function and $j_1(x)$ is a spherical Bessel function. $\psi_0(\alpha, \beta)$ is defined and evaluated in the Appendix along with some other related integrals. Conventional notation is employed for the various special functions encountered [15]. Details of the integrations involved will be presented elsewhere [16] (see [2], Appendix).

3. Intermediate magnetic field strength

The de Haas–van Alphen (DHVA) oscillatory parts of R which are characteristic of intermediate magnetic field strengths may be obtained from (4) by using a Laurent series expansion to represent the isolated essential singularities of the s-integrand at $s_1 = 1\pi i/u$, $1\pi i/u'$ to execute the s-integral in closed form. The u-integral has also been performed, and for $\alpha = 1$ (spin splitting the same as Landau level separation) and $\xi \gg 1$ ($\zeta \gg \omega_c$), we obtain the de Haas–van Alphen oscillatory part of R as $R_{\rm cl}^{\rm DHVA} + R_{\rm QI}^{\rm DHVA}$, where

$$R_{\rm cl}^{\rm DHVA}(r_1, r_s; \Omega = 0) \frac{1}{\pi^4}(m^*)^{5/2}(\mu_0^* H)^{3/2}\sqrt{2}J_0(k_{\rm F}\bar{R})$$

$$\times \sum_{l=1}^{\infty}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} l^{-3/2}\{R_{1,2_m}^{-1}\cos[l\pi\xi^+(a|z_{1,2_n}|^2/l\pi) + \pi/4]$$

$$+ R_{1,2'_m}^{-1}\cos[l\pi\xi^+(a|z_{1,2'_n}|^2/l\pi) + \pi/4]\} \qquad (7a)$$

$$R_{\rm QI}^{\rm DHVA}(r_1, r_2; \Omega = 0) = -\frac{1}{\pi^4}(m^*)^{5/2}(\mu_0^* H)^{3/2}\sqrt{2}J_0(k_{\rm F}\bar{R})$$

$$\times \sum_{l=1}^{\infty}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} l^{-3/2}\{R_{1,2'_m}^{-1}\cos[l\pi\xi^+(a|z_{1,2'_n}|^2/l\pi) + \pi/4]$$

$$+ R_{1,2'_m}^{-1}\cos[l\pi\xi^+(a|z_{1,2'_n}|/l\pi) + \pi/4]\}. \qquad (7b)$$

4. Quantum strong-field limit

For the quantum strong-field limit, in which all electrons are confined to the lowest Landau eigenstate with $\xi < 1$, the exponents of (4) may be simplified noting that $\coth(su) \to 1$, etc., and the s- and u-integrals are readily carried out with the result $R = R_{\rm cl}^{\rm QSF} + R_{\rm QI}^{\rm QSF}$ where ($\xi' = \xi + \alpha - 1$, $k'_{\rm F} = 2(a\xi')^{1/2}$)

$$R_{\rm cl}^{\rm QSF}(r_1, r_2; \Omega = 0) = (\mu_0^* H)^2(m^*/\pi)^3\,{\rm e}{-2a\bar{R}^2}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}$$

$$\times \{{\rm Si}[k_{\rm F'}(|z_{1,2_m}| + |z_{1,2_n}|)] + {\rm Si}[k_{\rm F'}(|z_{1,2'_m}| + |z_{1,2'_n})]\} \qquad (8a)$$

$$R_{\rm QI}^{\rm QSF}(r_1, r_2; \Omega = 0) = -2(\mu_0^* H)^2(m^*/\pi)^3\,{\rm e}^{-2aR^2}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}{\rm Si}[k'_{\rm F}(|z_{1,2_m}| + |z_{1,2'_n}|)]. \qquad (8b)$$

5. Conclusions

The results presented above explicitly exhibit the effects of multiple boundary reflections of electron wavefunctions on Friedel density oscillations in various regimes of quantising magnetic field strength. Our analysis of the density perturbation $\rho(1) = R(r_1, r_2; \Omega){\rm e}^{-i\Omega t_1}$ in the static limit $\Omega \to 0$ incorporates both 'classical' and 'quantum interference' contributions due to interference between incoming and reflected electron waves at interfaces. Multiple-boundary-reflection effects arise here directly from the superposition of a series of infinite-space-image Green's functions to impose the boundary condition of specular reflection (infinite barrier model) at the two faces of the infinite-width slab, film or quantum well.

Our use of closed-form integral representations, for both the magnetic field Green's function and for the Landau quantised electron density perturbation response function $R(1,2)$ in real-space representation (mainly in the degenerate case) have completely circumvented explicit reference to sums over Landau levels: The attendant Landau state matrix elements have been effectively evaluated explicitly in our work. Multiple-boundary-reflection effects in Friedel density oscillations have been determined explicitly here for low–intermediate magnetic field strengths, exhibiting de Haas–van Alphen oscillatory behaviour, and for the quantum strong field limit (all electrons in lowest Landau state). These results provide a convenient basis for a further analysis of the Friedel oscillation of static shielding of an arbitrary impressed potential subject to multiple-boundary-reflection effects at the two bounding surfaces of a solid state plasma in a quantising magnetic field. Moreover, this work concerning the density perturbation response function will be useful in the determination of the indirect-exchange RKKY interaction energy between two spins coupled via hyperfine interaction mediated by the conduction electrons of a finite metal film in a magnetic field [17]. The use of Mössbauer spectroscopy to measure hyperfine fields in bulk samples is well established. Its application to thin films should permit a measurement of the RKKY interaction which may be readily predicted from this work as a function of magnetic field strength, including the role of all multiple-wave-function reflections from the two film boundaries.

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Appendix

The following list of integrals and formulas is recorded here for the reader's convenience.

$$J_\nu(2(a\zeta)^{1/2}) = \left(\frac{a}{\zeta}\right)\nu/2 \int_{-i=+\delta}^{i=+\delta} \frac{ds}{2\pi i} e^{s\zeta} \frac{e^{-a/s}}{s^{\nu+1}} \qquad \mathrm{Re}\,\nu > -1 \tag{A1}$$

$$\varphi_\nu(\alpha,\beta) \equiv \int_0^1 \frac{du}{(uu')^{3/2}} \left(\frac{\alpha}{u'}+\frac{\beta}{u}\right)^{-\nu/2} J_\nu\left[\left(\frac{\alpha}{u'}+\frac{\beta}{u}\right)^{1/2}\right]$$

$$= (2\pi/\alpha\beta)^{1/2}(\alpha^{1/2}+\beta^{1/2})^{3/2-\nu} J_{\nu-1/2}(\alpha^{1/2}+\beta^{1/2}) \tag{A2}$$

$$\Psi_0(\alpha,\beta) \equiv \int_0^1 du\, u^{1/2}(u')^{-3/2} J_0\left[\left(\frac{\alpha}{u'}+\frac{\beta}{u}\right)^{1/2}\right]$$

$$= 2\{\alpha^{-1/2}\cos(\alpha^{1/2}+\beta^{1/2}) + \mathrm{Si}[\tfrac{1}{2}(\alpha^{1/2}+\beta^{1/2})]\} \tag{A3}$$

$$C_0(\alpha, \beta) \equiv \int_0^1 \frac{\mathrm{d}u}{(uu')^{1/2}} J_0\left[\left(\frac{\alpha}{u'} + \frac{\beta}{u}\right)^{1/2}\right] = -2\,\mathrm{Si}[(\alpha^{1/2} + \beta^{1/2})/2]. \tag{A4}$$

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