Electron states near a curved interface

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The quasi-two-dimensional quantum states of an electron near a curved interface between two media are studied. It is shown that the potential of the image forces of a point charge that is"pressed" against the curved interface contains a part that depends on the surface curvature and goes as $H\ \ln|zH|$, where $H(\mathbf{r}_s)$ is the mean curvature of the surface, and z is the distance from it. An equation is obtained for the wave function of an electron moving along the curved interface. Near individual irregularities two-dimensional localization is possible. The bound states near the extremum points of the curvature are described by the equation for a two-dimensional anisotropic oscillator. It is shown that in an arbitrarily strong magnetic field the degree of anisotropy of the ground state of such an oscillator approaches a constant limit. The application of the results to irregularities on heterojunction boundaries, on MIS structures, and on surfaces of solid hydrogen and neon, including hydrogen dust particles in interstellar space, are discussed.

1. INTRODUCTION

The electronic states near the interface between two media have been the object of intensive study in recent years. As examples we may cite electrons above the surface of liquid helium[1,2] or semiconductor electrons in metal-insulator-semiconductor structures or heterostructures. Most of the investigations in this field have been focused on the case of a plane interface. All the same, there is interest in studies of curved surfaces. In this case the energy of an electron depends on its position on the surface so consequently phenomena such as two-dimensional localization, variation in the structure of the spectrum of the magnetic levels, etc., are possible. The curvature of the surface of liquid helium in the presence of an external constraining electric field has been the subject of many investigations (see, e.g., the review, Ref. 1). In the case of semiconducting films of variable thickness, analogous problems have been studied in Refs. 3 and 4.

There is, however, another important (and in a certain sense a general mechanism through which surface curvature has an effect on the near-surface electrons. This mechanism is associated with the fact that the image forces depend on the curvature of the surface. In particular, this effect is important for understanding the structure of the bound states on small particles (grains of solid hydrogen in interstellar space,[5,6] liquid helium droplets,[6,7] or semiconductor particles embedded in an insulator or another semiconductor), or surface irregularities (cryogenic insulators-solid hydrogen[8] or neon-heterojunctions, or MIS structures), that occur naturally or are produced artificially. These states may govern the absorption, emission, and scattering spectra of electromagnetic waves (and their polarization) and the characteristic cyclotron resonance features that appear in the kinetic characteristics.

Our investigation focuses on the role of the image forces in the formation of the bound electron states at arbitrary curved interfaces between two media, both with and without the presence of a magnetic field.

2. IMAGE FORCE POTENTIAL NEAR A CURVED INTERFACE

Below we will confine the discussion solely to the case where the electron is localized (by image forces or by any other kind of force) at small distances from the interface, i.e., $\bar{z}$, its average distance from the interface, is much smaller than the characteristic radius of curvature R_0 of the surface:

$$\xi=\bar{z}/R_0\ll 1, \quad R_0\sim R_1(\mathbf{r}_s),\ R_2(\mathbf{r}_s). \tag{1}$$

Here $R_i(\mathbf{r}_s)$ is the principal radius of curvature at the point $\mathbf{r}_s$ of the surface.

We shall now find the potential energy of a point charge above the surface of the interface. By virtue of inequality (1) the potential energy of the image forces in the leading approximation is given by the expression for a plane surface:

$$u_0(z)=\frac{\alpha e^2}{4z}, \quad \alpha=\frac{\varepsilon_2-\varepsilon_1}{\varepsilon_2(\varepsilon_2+\varepsilon_1)}, \tag{2}$$

where z is the distance to the surface along its normal, e is the electron charge, and ε_1 and ε_2 are the dielectric constants of the two media (with the electron being in medium 2). An important consideration is that $u_0(z)$ does not depend on the point of the curved surface. Therefore the correction that we derive below to (2) for the curvature will also be a leading term that determines the motion of the electron over the surface.

Let a normal, dropped from the position $\mathbf{r}_0$ of a charge to the surface, intersect the surface at the point $\mathbf{r}_s$. Let us construct through this point a tangent plane on which the x and y axes are directed along the tangents to the principal normal sections. The equation of the surface near the point $\mathbf{r}_s$ can be written in the form

$$z+F(x,\ y)=0. \tag{3}$$

Transforming to the coordinate system $x'=x$, $y'=y$, $z'=z+F(x,y)$ converts the interface to a plane, and Poisson's equation takes the form

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$$\Delta\varphi+\hat{L}\varphi=\frac{4\pi e}{\varepsilon_2}\delta(\mathbf{r}-\mathbf{r}_0),$$
$$\hat{L}=\left(F_{xx}+F_{yy}+2F_x\frac{\partial}{\partial x}+2F_y\frac{\partial}{\partial y}\right)\frac{\partial}{\partial z}+(F_x^2+F_y^2)\frac{\partial^2}{\partial z^2} \quad (4)$$

(analogously to Ref. 4). In the immediate vicinity of the point $\mathbf{r}_s$

$$F(x,\ y)=x^2/R_1(\mathbf{r}_s)+y^2/R_2(\mathbf{r}_s),\quad x,\ y\ll R_i(\mathbf{r}_s). \quad (5)$$

After $F(x, y)$ has been substituted from (5) into (4) the additional terms $\hat{L}(\varphi)$ can be treated by perturbation theory. Using as the zero order approximation the Green's function of the problem of the planar interface, finding $\varphi(\mathbf{r}, \mathbf{r}_0)$, and then calculating the potential energy of the image forces, we obtain to within terms of order ξ)

$$u(\mathbf{r})=u_0(z)+u_1(z,\ \mathbf{r}_s),$$
$$u_1(z,\ \mathbf{r}_s)=\alpha e^2H(\mathbf{r}_s)\ln|zH(\mathbf{r}_s)|, \quad (6)$$

where the mean curvature of the surface at the point $\mathbf{r}_s$ is

$$H(\mathbf{r}_s)=\tfrac{1}{2}[R_1^{-1}(\mathbf{r}_s)+R_2^{-1}(\mathbf{r}_s)]. \quad (7)$$

We note that $u_1/u_0\propto\xi\ \ln\xi$, i.e., the correction term is not analytic in ξ.

3. EQUATION FOR THE WAVE FUNCTION AND TWO-DIMENSIONAL LOCALIZATION

The Schrödinger equation for a near-surface electron is written

$$-\frac{\hbar^2}{2m_e}\Delta\Psi+[u_0(z)+v(z)+u_1(z,\mathbf{r}_s)]\Psi=E\Psi. \quad (8)$$

Here m_e is the effective mass, $v(z)$ is a constraining potential of a nature different from that of the image force (if such exists). It should be noted that in the general case this potential also depends on $\mathbf{r}_s$. However, in what follows we shall limit the treatment to the case in which the surface $z=0$ is an equipotential for the external constraining electric field (if there is one; see e.g., Fig. 2). As regards short-range constraining potentials, their possible anisotropy leads to corrections proportional to ξ, which, in the leading approximation, may be neglected (in comparison to $\xi\ \ln\xi$ for the long-range image forces.

In Eq. (8) (provided ξ is small) we can decompose the motion of the electron into components perpendicular and parallel to the surface:

$$\Psi(\mathbf{r})=\chi_0(z)\psi(\mathbf{r}_s),\quad E=E_0+E_s, \quad (9)$$

where $\chi_0(z)$ and E_0 are taken from the solution to the planar interface problem (the electron is in the lowest "transverse" state). We shall assume that the curvature of the surface is so gentle that $R_0\gg a=\hbar^2/2m_e e^2\alpha$, where a is the effective Bohr radius associated with the image forces (when there is no additional constraining potential $v(z)$ we have $a\sim\bar{z}$ and this condition reduces that given above, namely, $\xi\ll1$). Then, averaging (8) over z with the use of $\chi_0(z)$ we obtain the leading approximation

$$-\frac{\hbar^2}{2m_e}\Delta_2\psi+u(\mathbf{r}_s)\psi=E_s\psi, \quad (10)$$
$$u(\mathbf{r}_s)=\alpha e^2H(\mathbf{r}_s)\ln|\bar{z}H(\mathbf{r}_s)|,$$

where $\Delta_2(\mathbf{r}_s)$ is the two-dimensional Laplacian operator on the surface, where the form of this operator depends on the shape of the surface and on the coordinate system, and E_s is the energy of motion along the surface.

Equation (10) describes the motion of a quasi-two-dimensional electron in the field of the image force above a surface of arbitrary shape, and of course, it does not admit of a general solution. We shall consider the most interesting special cases, limiting the problem to the localization of an electron near a particular irregularity, in the region of which the curvature is an extremum (a minimum for $\varepsilon_1>\varepsilon_2$ or a maximum for $\varepsilon_1<\varepsilon_2$).

1. Deep smooth well (radius of localization $l\ll L$). Here

$$L=\left[\frac{1}{u(\mathbf{r}_{sm})}\int d^2r_s u(\mathbf{r}_s)\right]^{1/2} \quad (11)$$

is the characteristic "average" size of the well. In this case the electron is localized in the neighborhood of the point $\mathbf{r}_{sm}$—the extremum of $H(\mathbf{r}_s)$ and in Eq. (10) we can expand in the small quantity $|\mathbf{r}_s-\mathbf{r}_{sm}|\ll R_0$. Here $\Delta_2(\mathbf{r}_s)$ can be conveniently written in the local coordinates

$$\Delta_2=R_1^{-2}(\mathbf{r}_s)\frac{\partial^2}{\partial\theta_1^2}+R_2^{-2}(\mathbf{r}_s)\frac{\partial^2}{\partial\theta_2^2} \quad (12)$$

where the θ_i are the polar angles in the planes of the corresponding transverse cross sections (Fig. 1), and $\theta_i\ll1$. Keeping only terms of second order in θ_i in the expansion of $u(\mathbf{r}_s)$ and zero order terms in θ_i in the expansion of $\Delta_2(\mathbf{r}_s)$, (i.e., to accuracy of the order $1/R_0$), and introducing the Cartesian coordinates $x_i=R(\mathbf{r}_{sm})\theta_i$, we obtain an oscillator equation of the type

$$-\frac{\hbar^2}{2m_e}\left(\frac{\partial^2\psi}{\partial x_1^2}+\frac{\partial^2\psi}{\partial x_2^2}\right)+\frac{1}{2}g_{ik}x_ix_k\psi=\Delta E\psi,$$
$$\Delta E=E_s-u(\mathbf{r}_{sm}), \quad (13)$$
$$g_{ik}=\alpha e^2\ln|\bar{z}H(\mathbf{r}_{sm})|\left.\frac{\partial^2H}{\partial x_i\,\partial x_k}\right|_{\mathbf{r}_s=\mathbf{r}_{sm}}.$$

Reducing the tensor g_{ik} to the principal axes x and y (principal values g_1 and g_2), we can obtain the solution in the form of the wave functions of a two-dimensional oscillator:

$$\psi_{nm}(x,y)=(\pi l_1l_2\cdot2^{n+m}n!m!)^{-1/2}H_n\left(\frac{x}{l_1}\right)H_m\left(\frac{y}{l_2}\right)$$
$$\times\exp\left(-\frac{x^2}{2l_1^2}-\frac{y^2}{2l_2^2}\right). \quad (14)$$

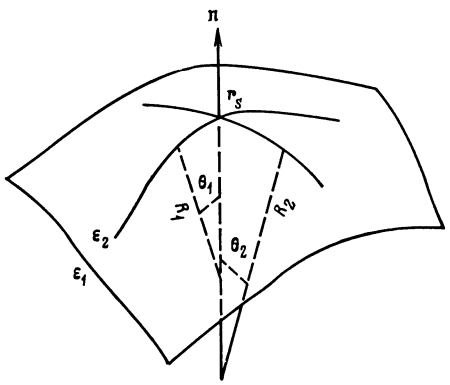

FIG. 1.

Here the $H_n(z)$ are Hermite polynomials, and $l_i = (\hbar^2/m_e g_i)^{1/4}$. The energy spectrum is given by the expression

$$\Delta E_{nm} = \hbar\omega_1(n+1/2) + \hbar\omega_2(m+1/2), \quad \omega_i = (g_i/m_e)^{1/2}. \quad (15)$$

Let us turn now to the conditions for the applicability of this theory. For a sufficiently smooth irregularity there is one characteristic dimension R_0, such that $L \sim R_0$ and $\partial/\partial x_i \sim 1/R_0$, and so $l^4 \sim l_i^4 \sim aR_0^3/\ln(R_0/\bar{z})$. Thus, the condition $l \ll L$ reduces to $R_0 \ln(R_0/\bar{z}) \gg a$, i.e., it is satisfied everywhere (for these irregularities) in the region of applicability of (10).

For the typical case of an arbitrarily oriented ellipsoidal irregularity (concave for $\varepsilon_1 > \varepsilon_2$ or convex for $\varepsilon_1 < \varepsilon_2$) with semiaxes $a_1 \leqslant a_2 \leqslant a_3$ the electron is localized near the pole of greatest curvature (i.e., near axis 3). In this case in formulas (14) and (15)

$$g_1 = \left| \frac{\alpha e^2 a_3}{2a_1^2 a_2^2}\left(1 - \frac{a_3^2}{a_1^2}\right)\left(1 + 3\frac{a_2^2}{a_1^2}\right)\ln\left[\frac{\bar{z}a_3}{2}\left(\frac{1}{a_1^2} + \frac{1}{a_2^2}\right)\right]\right|, \quad (16)$$

and g_2 is obtained from g_1 by the interchange of axes $1 \rightleftarrows 2$.

We emphasize that our results also apply in a natural way to the case of a closed surface (a droplet, a small particle, or an inclusion). Here the value of L is limited by the particle size. For instance if the latter ellipsoidal, as described above, and $\varepsilon_1 > \varepsilon_2$, then the electron (which is outside the particle) is localized in the "flattest" region, near axis 1, so that in formula (16) the indices should be interchanged $1 \rightleftarrows 3$.

2. Shallow well (the opposite limiting case $l \gg L$). In this case the longitudinal dimension of the well is much less than $R_i(\mathbf{r}_{sm})$. As is well known, for two-dimensional motion a bound state also exists in this case,[10] with the energy level and the wave function outside the (in general, asymmetric) well given by the expression

$$|E| = \frac{\hbar^2\varkappa^2}{2m_e} \sim \frac{\hbar^2}{m_e L^2}\exp\left[-\frac{\hbar^2}{m_e}\left(\int u(\mathbf{r}_s)\,d^2r_s\right)^{-1}\right], \quad (17)$$

$$\psi(\mathbf{r}_s) \sim K_0(\varkappa r_s) \quad (r_s \gg L), \quad (18)$$

where K_0 is the modified Bessel function of the second kind.

The criterion for the applicability of (17) and (18) is obtained from the requirement $\varkappa L \ll 1$, which is equivalent to the condition that the exponent in (17) be small:

$$\frac{m_e}{\hbar^2}\int u(\mathbf{r}_s)\,d^2r_s \ll 1, \quad (19)$$

i.e., in every case the condition $L^2 \ln(R_0/\bar{z}) < R_0 a$ must hold.

4. STATES IN A MAGNETIC FIELD

In the case of a magnetic field we make the usual substitution $i\hbar\nabla \to i\hbar\nabla + (e/c)\mathbf{A}$. We choose a special gauge in which $\mathbf{A}(\mathbf{r}_s)\cdot\mathbf{n}(\mathbf{r}_s) = 0$, where $\mathbf{n}(\mathbf{r}_s)$ is the normal to the surface. Then in Eq. (10) Δ_2 should be replaced by the operator

$$\sum_{i=1}^{2}\left(\frac{1}{h_1h_2}\frac{\partial}{\partial x_i}\frac{h_1h_2}{h_i} - \frac{ie}{c\hbar}A_i\right)\left(\frac{1}{h_i}\frac{\partial}{\partial x_i} - \frac{ie}{c\hbar}A_i\right), \quad (20)$$

where h_i are the Lamé coefficients of the curvilinear orthogonal coordinate system on the surface.

Let us consider the simplest case. A uniform magnetic field $\mathscr{H}$ is directed along the normal to the surface at the point $\mathbf{r}_{sm}$. As we did before, we shall select a system of local coordinates (Fig. 1) at the point $\mathbf{r}_{sm}$ in such a way that in the new coordinates x and y the tensor g_{ik} defined by formula (13) is diagonal. It can be shown that in this case the vector potential chosen in the usual form $\mathbf{A}(\mathscr{H}y, 0, 0)$ in the region of localization satisfies the gauge condition $\mathbf{A}\cdot\mathbf{n} = 0$ accurate to terms in l/R_0, and to the same degree of accuracy we obtain the equation for the electron wave function

$$\frac{\hbar^2}{2m_e}\left[\left(i\frac{\partial}{\partial x} - y/l_{\mathscr{H}}^2\right)^2 - \frac{\partial^2}{\partial y^2}\right]\psi + \frac{1}{2}(g_1x^2 + g_2y^2)\psi = \Delta E\psi, \quad (21)$$

which describes an anisotropic two-dimensional oscillator in a magnetic field: here $l_{\mathscr{H}} = (c\hbar/e\mathscr{H})^{1/2}$ is the magnetic length.

Equation (21) is most conveniently solved by transforming to a Fourier representation in x and subsequently diagonalizing the dynamic matrix. The frequencies thus obtained

$$\Omega_{1,2} = 1/2[(\omega_1+\omega_2)^2 + \omega_c^2]^{1/2} \pm [(\omega_1-\omega_2)^2 + \omega_c^2]^{1/2} \quad (22)$$

determine the electron energy spectrum:

$$\Delta E = \hbar\Omega_1(n_1 + 1/2) + \hbar\Omega_2(n_2 + 1/2). \quad (23)$$

Here $\omega_c = e\mathscr{H}/m_e c$ is the cyclotron frequency and ω_i is defined in (15). The expressions for the wave function $\psi_{n_1n_2}(x, y)$ are rather cumbersome so we shall write down only the wave function for the ground state

$$\psi_{00}(x, y) = \left[\frac{\pi l_1 l_2(\omega_1+\omega_2)}{\Omega_1+\Omega_2}\right]^{-1/2} \times \exp\left[-\frac{\Omega_1+\Omega_2}{2l_{\mathscr{H}}^2\omega_c(\omega_1+\omega_2)}(\omega_1x^2 + \omega_2y^2) + \frac{i\omega_1xy}{l_{\mathscr{H}}^2(\omega_1+\omega_2)}\right]. \quad (24)$$

The asymmetric form of the phase factor is due to our choice of the gauge of the vector potential. In the cylindrical gauge $\mathbf{A}(\mathscr{H}y/2, \mathscr{H}x/2, 0)$ this factor takes the form

$$\exp[i(\omega_1-\omega_2)xy/2l_{\mathscr{H}}^2(\omega_1+\omega_2)].$$

It is interesting to note that even in the limit of large fields $l_i/l_{\mathscr{H}} \to \infty$ the symmetrized function $\psi_{00}(x, y)$ does not go over to the known solution for an electron in a magnetic field,[10] $n_\rho = m = 0$. This is because the anisotropic potential of the oscillator lifts the infinite degeneracy in negative values of the momentum m in Ref. 10.

Here the form of the wave function depends only on the ratio ω_1/ω_2, which characterizes the degree of anisotropy of the potential.

The anharmonic terms that were discarded in the derivation of (21) give nonequidistant corrections to the energy levels proportional to $\hbar\Omega(1/R_0)^2n^2$. Their exact form for the special case of a spherical particle ($\omega_1 = \omega_2 = 0$) is given in our previous paper.[6]

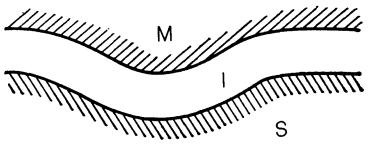

FIG. 2.

5. CONCLUSIONS

In conclusion we shall discuss the possibilities of observing these states experimentally and the choice of the physical system that is most appropriate for this purpose. Let us note first of all that our treatment is valid for the condition $R_0 \gg \bar{z}$, where R_0 is the characteristic radius of curvature of the surface and $\bar{z}$ is the mean distance from it to the electron. Since in every case $\bar{z} \gg 1$ Å, it is necessary that $R_0 \gtrsim 100$ Å, so that the characteristic energy is $E_s \sim 10$ K.

By way of example let us cite some systems that are suitable for experimental study of these states:

1. The surface of a cryogenic insulator—solid hydrogen or neon. In this case the electron is constrained to the surface by the image forces themselves and it is localized near small cavities on a plane surface[8] or at regions of low curvature on the hydrogen particles.

2. Natural or artificial irregularities of the interface (heterojunction) between two semiconductors or small inclusions of one semiconductor in another.

3. Curved MIS structures of the kind shown in Fig. 2.

We shall give a specific estimate for the case of solid hydrogen. For the ground state of the transverse motion $E_0 \sim 250$ K and $\bar{z} \sim 20$ Å. Oscillator states exist for irregularities with $R_0 \gtrsim 300$ Å, for which $\hbar\omega_i \lesssim 5$ K. A marked change in these states occurs in magnetic fields as low as $\mathscr{H} \sim 10^4$ G ($l_{\mathscr{H}} \sim 250$ Å).

Direct experimental observation of these states is possible in the first place through the effects of their resonance interaction with electromagnetic waves (in the wavelength 0.5–1 mm) or with electron beams (of course, in this case the irregularities should be about the same size). The positions of the absorption, emission, and Raman scattering spectral lines and their fine structure [determined by the anharmonic corrections to (13)] carry information on the size and shape of the irregularities, while the orientation of the principal

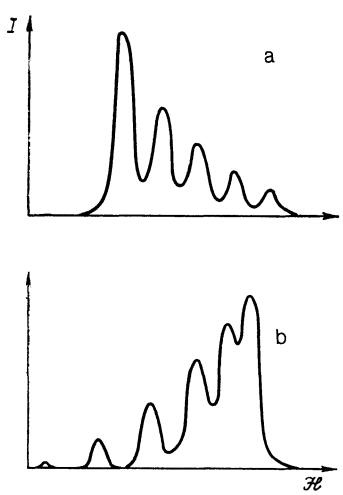

FIG. 3. Qualitative picture of the structure of the "cyclotron" resonance lines: a) $\Omega_1(\mathscr{H})$; b) $\Omega_2(\mathscr{H})$.

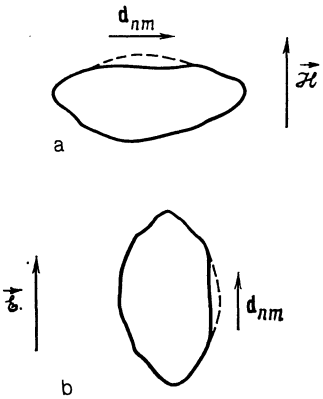

FIG. 4. Preferential orientation of dipole matrix element vectors (of an electron on a hydrogen dust particle) relative to the external magnetic field (a) and electric field (b).

axes of the tensor g_{ik} determines the polarization.

The features of resonance absorption in a magnetic field are interesting. The transition frequencies $\Omega_i(\mathscr{H})$ depend on $\mathscr{H}$ in a very nonlinear way. In the limit of strong fields ($\omega_c \gg \omega_i$), $\Omega_1 \to \omega_c$ and $\Omega_2 \sim \omega_1\omega_2/\omega_c \ll \omega_i$ and the latter (Ω_2) depends anomalously on the magnetic field ($\propto \mathscr{H}^{-1}$). Taking the anharmonicity into account brings about a splitting of both resonance lines into $\bar{n} \sim 1 + kT/\hbar\Omega_i$ peaks equidistance in $\mathscr{H}$ and $\mathscr{H}^{-1}$, respectively, or (in the case of sufficient variation in the irregularity sizes) an inhomogeneous line broadening (Fig. 3).

Let us discuss, finally, the possible connection, pointed out by Chaikin,[5] between electron states localized on interstellar dust particles and the propagation of electromagnetic waves in interstellar space. The orientation of particles of irregular shape in an external constant field (Fig. 4) leads to the result that the radiation associated with the oscillator transitions of the type discussed above (in the wavelength range $\lambda \gtrsim 10$ cm^{-1}) is preferentially polarized in the direction of the electric field (or pependicular to the magnetic field).

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