Spin-density-wave instability in wide parabolic quantum wells

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Calculations of electrons in a remotely doped wide parabolic quantum well, in the presence of a strong in-plane magnetic field, using a modified Hartree-Fock approximation with a point-contact exchange interaction, support the idea that a spin-density-wave state may occur in an experimentally accessible range of parameters. Electrical transport in the spin-density-wave state is expected to be finite at zero temperature, but highly anisotropic, with a low resistivity for currents perpendicular to the magnetic field.

I. INTRODUCTION

Over the years, it has been proposed that an interacting three-dimensional (3D) electron system in a uniform positive background, subjected to a large applied magnetic field, must undergo á phase transition at low temperatures to some kind of state with a broken translational symmetry.[1-4] In the limit of very strong magnetic fields, the ground state is clearly a Wigner crystal.[2] For intermediate values of the magnetic field, however, other types of ground state may be possible. One of the most interesting of these is the Celli-Mermin spin-density-wave (SDW) state,[1] which would have very anisotropic transport properties[3]—a vanishing electrical resistance perpendicular to the magnetic field **B** and a diverging resistance parallel to **B**.

Attempts to look for the hypothetical broken symmetry states in 3D doped semiconductors seem to be thwarted by the strong interaction of the carriers with the neutralizing charged impurities which are inevitably present.[5]

Recently, however, a man-made structure was suggested,[3,6,7] in which there exists a thick (>1000 Å) and uniform layer of high-mobility electrons. The idea is to grow a compositional wide parabolic quantum well (WPQW) of $Ga_{1-x}Al_xAs$ bounded by $Ga_{1-y}Al_yAs$. If Δ_1 is the height of the parabolic well, W the width of the well, and ϵ the dielectric constant which is assumed constant across the well, this potential is similar to the potential created by a uniform slab of positive charge of density $n_0=2\epsilon\Delta_1/W^2e^2\pi$. Electrons trapped in the well will screen this fictitious charge density and will form a uniform layer of three-dimensional density n_0. (See Fig. 1.) We define the fractional occupation of the WPQW as $\eta=n_s/n_0W$, where n_s is the number of electrons per unit area. An increase of η, in the range $0<\eta<1$, will produce a linear increase of the thickness of the electron layer. Since the donors are removed several hundred angstroms from the WPQW, the electron-impurity interaction is significantly smaller in these systems than in the usual doped semiconductors. Such WPQW's were recently grown,[6,7] and magnetotransport experiments on these systems reveal that they hold a high-mobility, thick slab of electron gas.

The question then arises whether the geometries that can be achieved in practice are in fact thick enough that one would expect to see some manifestation of the behavior of the ideal three-dimensional system in a strong magnetic field.

It is relatively clear that in the limit of strong magnetic fields, the ground state of the WPQW should be some kind of (disordered) Wigner crystal. Just as for the infinite 3D case, one can argue that in the limit of $B\rightarrow\infty$ the electron states are easily localized in the direction perpendicular to **B**, and the kinetic energy in the direction parallel to **B** is sufficiently small that some form of localization should occur in that direction as well. In a finite parabolic well, then, without impurities, one would expect a crystalline ground state in which there are several layers of electrons in the z direction (perpendicular to the plane of the well) with a periodic structure in

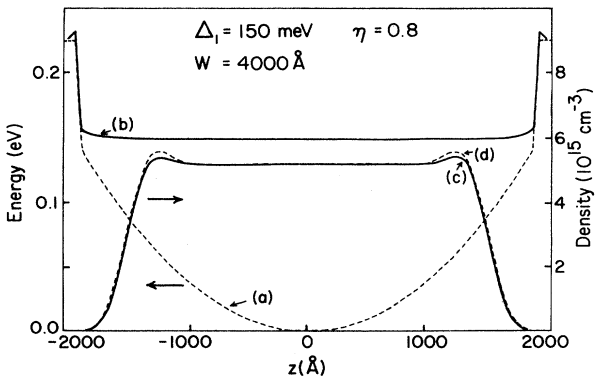

FIG. 1. Potential and charge density in a 4000-Å-wide parabolic well in $Al_xGa_{1-x}As$ for the case of filling factor $\eta=0.8$ and an applied magnetic field $B=1$ T, parallel to the well. Curve (a) shows the bare potential $V(z)$ for the well, curve (b) shows the self-consistent potential in the Hartree approximation $V(z)+V_H(z)$. The solid curve (c) shows the electron density in the Hartree approximation, while the dashed curve (d) is the density obtained with a dimensionless exchange parameter of $\lambda=0.63$. The depth of the bare well is $\Delta_1=150$ meV.

the x and y directions. The detailed form of the crystal would depend on the parameters of the well and the direction of the applied magnetic field. In practice, the potential of the charged impurities outside the well and of residual impurities inside the well would no doubt lead to a destruction of the ideal periodicity in the direction parallel to the well and would presumably lead to a smearing of the transition into a Wigner-crystal state; but, the qualitative properties should not be greatly affected.

Although there are many interesting questions concerning the onset and properties of a Wigner-crystal state, in the present paper we concentrate on the more exotic possibility, the Celli-Mermin SDW state, in situations where there is a magnetic field of intermediate strength, in a direction parallel to the plane of the sample. We recall that in one-dimensional systems, within a screened Hartree-Fock approximation, for any strength of the electron-electron repulsion, the formation of a sufficiently weak SDW costs less in kinetic energy than it gains in reduced potential energy as was first noted by Overhauser. In similar way, metals with a nesting Fermi surface, such as chromium, are unstable against the formation of a SDW. Celli and Mermin[1] showed that, due to the one-dimensional character of the 3D electron gas in the presence of a uniform magnetic field, the ground state of this system, at sufficiently low temperatures, is not the uniform state, and they proposed that for intermediate values of **B**, not so strong as to completely align the spins of the electrons, the ground state should have an SDW with wave vector **Q** directed along the field. We shall explore here the question of whether the electron layer in a WPQW is thick enough so that a similar SDW instability is expected, and we shall discuss some properties of the SDW state if it occurs.

II. DESCRIPTION OF THE MODEL

In a modified Hartree-Fock approximation, using a Coulomb interaction for the direct term and a contact interaction $v(\mathbf{r}-\mathbf{r}')=I\delta(\mathbf{r}-\mathbf{r}')$ for the exchange term, the eigenvalues and eigenstates of the WPQW with translational invariance in the x-y plane, and a magnetic field parallel to $\hat{\mathbf{x}}$, have the form

$$\Psi_{n,\mathbf{k},\sigma}(\mathbf{r})=\frac{e^{i(k_x x+k_y y)}}{\sqrt{S}}\Phi_{n,k_y,\sigma}(z)\ , \tag{1a}$$

$$E_{n,k_x,k_y,\sigma}=k_x^2/2m^*+\varepsilon^{\sigma}_{n,k_y}\ , \tag{1b}$$

where we have used the Landau gauge $\mathbf{A}=(0,-Bz,0)$, and $\Phi_{n,k_y,\sigma}(z)$ and $\varepsilon^{\sigma}_{n,k_y}$ are eigenstates and eigenvalues of the one-dimensional Hamiltonian:

$$H_{k_y,\sigma}=-\frac{1}{2m^*}\frac{\partial^2}{\partial z^2}+\frac{B^2}{2m^*}(z+z_0)^2+V_T(z)-g^*\mu_B B\sigma\ , \tag{2a}$$

$$z_0\equiv\frac{k_y c}{eB}\ , \tag{2b}$$

where $V_T(z)=V(z)+V_H(z)-In_{\sigma}(z)$. In these expressions, $V(z)$ is the bare potential of the WPQW, $V_H(z)$ is the Hartree potential arising from the Coulomb potential of the self-consistent electron density $n(z)$, $n_{\sigma}(z)$ is the density of electrons with an x component of spin $\sigma=\pm\frac{1}{2}$, μ_B is the Bohr magneton, g^* is the effective Landé factor, and m^* is the effective mass. We take $g^*=0.4$, and a constant effective mass and dielectric constant, $m^*=0.067$ and $\epsilon=12.5$, respectively, characteristic of GaAs. The positively charged donor impurities which are necessary to maintain charge neutrality (and to prevent the self-consistent potential from decreasing towards $-\infty$ outside the well) are represented in our model by two uniform positive layers of equal charge density, 200 Å thick, located just outside the well on either side. We have checked that our results for the electron layer are insensitive to the precise location of the positive charges, for reasonable choices of the parameters.

The one-dimensional Hamiltonian, Eq. (2), depends on k_y through the "center" of the orbit $z_0=l_m^2 k_y$, where l_m is the magnetic length. If z_0 is placed in regions where the $V_T(z)$ is constant, we recover the usual Landau levels, and the energy is independent of z_0, but the energy $\varepsilon^{\sigma}_{n,k_y}$ increases quadratically with k_y when the "guiding center" z_0 approaches the edge of the electron slab. In the WPQW, for a thin electron slab the magnetic orbits of the electrons feel both edges of $V_T(z)$, and $\varepsilon^{\sigma}_{n,k_y}$ is nearly quadratic in k_y. When the thickness of the electron slab increases, there appears as a region of almost flat dispersion between the zones of edge states. (See Fig. 2.) The separation between energy bands "centered" in the middle of the WPQW converges to the Landau-level separation, when the magnetic field or the thickness of the electronic sheet increases.

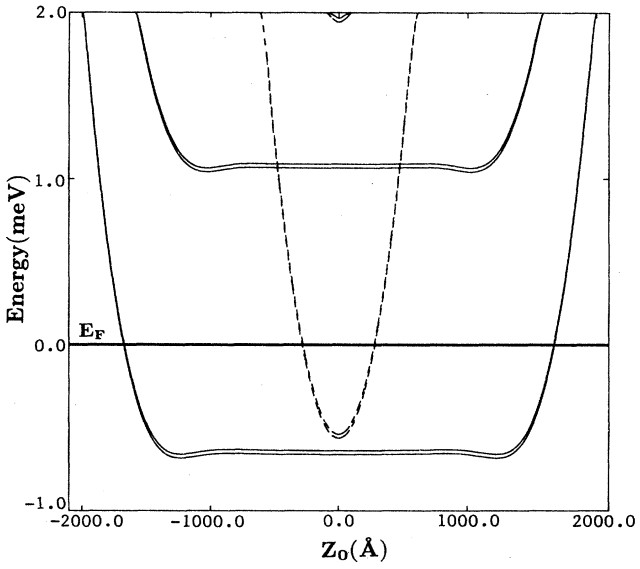

FIG. 2. Energy levels $\varepsilon^{\sigma}_{n,k_y}$ as a function of the "center" of the orbit z_0, for the case of $B=1$ T and $\lambda=0.63$. The solid line corresponds to $\eta=0.8$ and the broken to $\eta=0.1$. The energies are given with respect to the Fermi level. The parameters of the WPQW are the same as in Fig. 1.

As is shown in Fig. 1, in the Hartree approximation, the presence of a magnetic field does not affect the formation of a thick uniform slab of electronic charge in the WPQW. The inclusion of the point-contact "exchange interaction" produces an enlargement of the small oscillations that the charge density has in the Hartree approach. For larger interaction I, or larger magnetic fields, the density profile is no longer uniform, and strong oscillations appear in the z direction. In this limit there is also an increasing tendency to the formation of charge-density waves in the x-y plane, which we may interpret as an indication of Wigner crystallization. In the present paper, however, we are interested in SDW instabilities, and we restrict ourselves to magnetic fields and "exchange interactions" small enough such that the nearly uniform distribution of the charge in the z direction is stable. (See Fig. 1.)

We now calculate the SDW response function $\chi(z,Q_x)$, which gives the spin density at z, induced by a fictitious infinitesimal field $b_t e^{iQ_x x}\mathbf{u}_z$. A divergence of this function for some value of Q_x reveals the existence of a SDW instability with that wave vector. In the local Hartree-Fock approximation,[8] and in the case when only the lowest band is occupied, with both spin states present, the response function $\chi(z,Q_x)$ is obtained from

$$\chi(z,Q_x)=\frac{(g^*\mu_B)^2}{4S}\sum_{k_y,\sigma} P_{k_y}(z)X_\sigma(k_y,Q_x)\Gamma_\sigma(k_y,Q_x)\ , \tag{3}$$

$$\Gamma_\sigma(k_y,Q_x)=S_{k_y}+\sum_{k_y'} X_\sigma(k_y',Q_x)g(k_y',k_y)\Gamma_\sigma(k_y',Q_x)\ , \tag{4}$$

where Γ_σ is a vertex function and we use the definitions (f is the Fermi function)

$$X_\sigma(k_y,Q_x)\equiv-\sum_{k_x}\frac{f(\sigma,k_x,k_y)-f(-\sigma,k_x-Q_x,k_y)}{E_{k_x,k_y,\sigma}-E_{k_x-Q_x,k_y,-\sigma}}\ , \tag{5a}$$

$$P_{k_y}(z)\equiv\Phi^*_{k_y,\sigma}(z)\Phi_{k_y,-\sigma}(z)\ , \tag{5b}$$

$$g(k_y',k_y)\equiv\frac{I}{S}\int dz\ \Phi^*_{k_y,-\sigma}(z)\Phi^*_{k_y',\sigma}(z)\times\Phi_{k_y',-\sigma}(z)\Phi_{k_y,\sigma}(z)\ . \tag{5c}$$

$$S_{k_y}\equiv\int dz\ \Phi^*_{k_y,\sigma}(z)\Phi_{k_y,-\sigma}(z)\ . \tag{5d}$$

In order to obtain these equations, we have ignored the contribution of intermediate electron states which are not in the lowest-energy band. We believe that this is a very good approximation for the parameters of interest here.

In Fig. 3 we plot, for $B=1$ T, the response function in the case of noninteracting electrons, for two values of the occupation η. When $\eta=0.1$, the eigenvalues [Eq. (1b)] depend nearly quadratically on k_y and the response function is that of a 2D system. For thicker slabs ($\eta=0.8$) there is a large region where the eigenvalues are almost

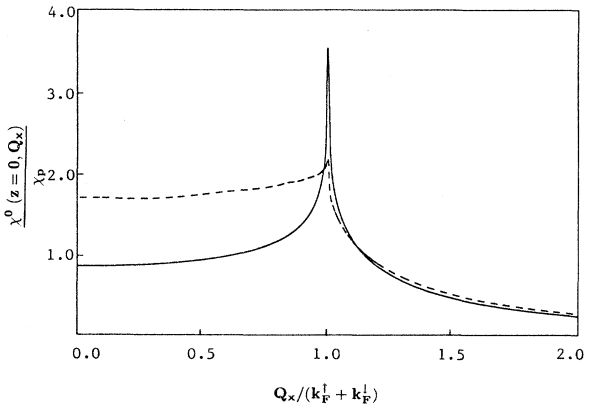

FIG. 3. Variation of the free-electron susceptibility $\chi(z=0,Q_x)$ as a function of Q_x, for a magnetic field of 1 T. The solid line corresponds to $\eta=0.8$ and the broken to $\eta=0.1$. The susceptibility is given in units of the Pauli susceptibility χ_p. The parameters of the WPQW are the same as in Fig. 1.

independent of k_y and the susceptibility resembles the one-dimensional response function. The finite size of the electron slab produces the result that instead of the logarithmic singularity in the response function, a finite maximum occurs at $Q_x\approx k_F^\uparrow+k_F^\downarrow$ (here $k_F^{\uparrow\downarrow}\equiv[2m^*(E_F-\varepsilon^{\uparrow\downarrow}_{k_y=0})]^{1/2}$). This maximum still leads to the result that when the exchange interaction is introduced, the first divergence of the response function occurs at $Q_x\approx k_F^\uparrow+k_F^\downarrow$. In the interacting system, we define a critical interaction I_c, which is the minimum value of I such that the vertex function (4) diverges. In Fig. 4, we show the variation of the dimensionless critical interaction $\lambda_c=I_c n_0/E_F^0$, where E_F^0 is the Fermi energy of a 3D electron gas of density $n_0=5.2\times10^{15}$ cm^{-3}, as a function of Q_x. The sharp dip that λ_c presents at $Q_x\approx k_F^\uparrow+k_F^\downarrow$ is an indication of a possible SDW instability with this wave vector. For fixed values of B and $Q_x=k_F^\uparrow+k_F^\downarrow$ the critical interaction strength λ_c tends approximately to a constant when the thickness becomes large. As seen in Fig. 5, the limit is reached for fractional occupation $\eta\geq0.4$ for $B=1$ T. The saturation of λ_c with η shows that the edge states lose their importance in the response function, as the thickness of the electron slab increases. The value of λ_c decreases with increasing B, roughly as $\lambda_c\simeq0.5/B^2$ (with B in teslas), due to the B^2 dependence of the free susceptibility in this quantum limit. However, as said above, for larger magnetic fields there is also an increasing tendency to other instabilities, such as a Wigner crystal, which may preempt the SDW transition.

In this model, we predict the existence of a SDW with a wave vector the sum of the Fermi wave vector of spin-up and spin-down electrons, whenever the value of the exchange interaction is bigger than a critical value λ_c. In order to apply our conclusions to an actual system, we must compare the values of λ_c with some estimated value of the dimensionless interaction $\lambda=In_0/E_F^0$. One possi-

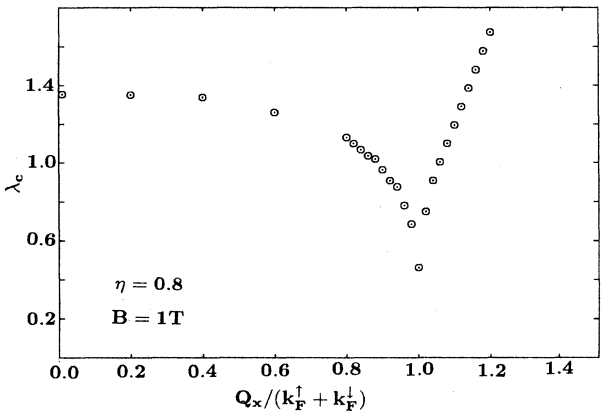

FIG. 4. Minimum values of the exchange interaction, λ_c, for the onset of an SDW instability at wave vector Q_x. A sharp dip occurs at the sum of the Fermi wave vectors for spin-up and spin-down electrons. The parameters of the WPQW are the same as in Fig. 1.

ble choice for λ is the long-wavelength limit of the Thomas-Fermi (TF) screened Coulomb potential, which gives $\lambda_{TF}=\frac{2}{3}$. Another choice is to use a typical value for the exchange-correlation potential[9] $\lambda_{xc}\simeq r_s/3$, where r_s is the Wigner-Seitz radius in units of the effective Bohr radius. For the parameters we are using, the tailored density corresponds to $r_s\approx 3.5$, so that both λ_{TF} and λ_{xc} are larger than the critical interaction strength λ_c. This supports the possible existence of a SDW instability in the WPQW.

Our calculations have been carried in the $T=0$ limit. The pertinent question is if the critical temperature T_c, at which the SDW instability disappears,[1,8] is high enough that the SDW becomes experimentally observable. In order to have an idea about the value of the critical temperature, we consider the case of a 3D electron gas of density n_0, where the "exchange interaction" is the long-wavelength limit of the static screened Thomas-Fermi potential. When a magnetic field is applied to this system, at zero temperature, the onset of a SDW ground state is indicated by the logarithmic singularity of the spin-density response function at the wave vector of the SDW. When considering the finite-temperature case this singularity is cut off by T. In this model, the weak-coupling regime,[1] and our quantum limit (only the lowest Landau level with both spins occupied) the critical temperature where the SDW instability disappears is

$$k_B T_c=\frac{8}{\pi}e^{\gamma}k_F^{\uparrow}k_F^{\downarrow}\frac{1}{2m^*}\exp\left[-\frac{(2\pi l_m)^2(k_F^{\uparrow}+k_F^{\downarrow})n_0}{2m^*E_F^0\lambda_{TF}}\right], \tag{6}$$

where γ is Euler's constant. With the parameters of our WPQW, we found values of T_c running between $T_c=0.25$ K ($B=1$ T) and $T_c=1.8$ K ($B=2$ T). Due to the exponential dependence of T_c on the parameters of the problem, these numbers are at best an order-of-magnitude estimate. Nevertheless, these temperatures are experimentally accessible and they suggest that a SDW may be observable under suitable conditions in a WPQW.

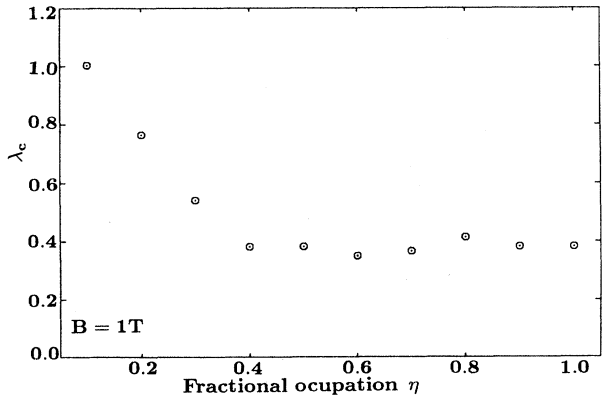

FIG. 5. Variation of the critical interaction, λ_c, for the onset of a SDW instability at wave vector $Q_x=k_F^{\uparrow}+k_F^{\downarrow}$, as a function of the fractional occupation η. The parameters of the WPQW are the same as in Fig. 1.

III. TRANSPORT PROPERTIES

The physical significance of the SDW instability can be understood by considering the form of the Fermi surface, for this WPQW, with and without the SDW, which are illustrated in Fig. 6. The flat portions of the Fermi surface in Fig. 6(a) are eliminated by the periodic potential of the SDW and are, therefore, absent in Fig. 6(b). States at the Fermi surface which remain in Fig. 6(b) are the states with larger values of k_y, corresponding to values of z_0 at either edge of the electron layer.

The group velocity $\mathbf{v}$ of an electron with wave vector (k_x,k_y) is given by the gradient of the energy respect to (k_x,k_y). It is clear that the states at the Fermi energy with $k_y>0$ in Fig. 6(b), corresponding to edge states with $z_0>0$, all have $v_y>0$, while the states at the opposite edge have $v_y<0$. The value of v_x depends on k_x, and both signs of v_x may be found at each edge of the layer.

Let us now consider the electrical-transport properties of the system in the presence of a SDW. We assume that the spin-density-wave structure is pinned by impurities, which couple to a charge-density wave induced at the first harmonic of the SDW by the intrinsic nonlinearity of the system. The random impurity potential will presumably lead to some distortion of the SDW, but let us assume, for the moment, there there are no dislocations in the SDW structure. The impurity potential will scatter electrons at the Fermi energy, on either side of the well, from one value of k_x to another. If the electron layer is thick compared to the magnetic length, however, there is very little overlap between the states from opposite sides of the layer, so that the impurities should produce very little scattering between these two sets of states. Since the states at a given edge carry a current of a definite sign in the y direction, they cannot be localized in that direction, and this probably implies that they must be extend-

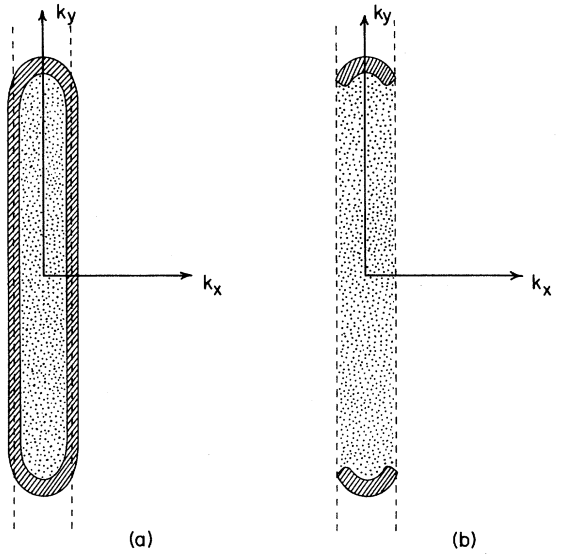

FIG. 6. (a) Schematic of Fermi surface in the absence of a SDW, for filling factor $\eta=0.8$ and $B=1$ T. (b) Schematic of Fermi surface in the presence of a SDW. Dark and light shading indicate regions where respectively one or both spin states are occupied. Dashed lines are the boundaries of the first Brillouin zone in the presence of the SDW. The overall shape of the Fermi surface in (a) and the flatness of the sides are obtained from our calculations, but the spin splitting has been greatly exaggerated for clarity.

ed also in the x direction.

In order for a current to be carried by the sample in the y direction, one must establish a difference in the electrochemical potential between the two sides of the electron layer (essentially a Hall voltage). The electrical current is then carried by a combination of two effects: an excess in charge carriers at the edge corresponding to a positive group velocity and a contribution from the $\mathbf{E}\times\mathbf{B}$ drift of electrons in the center of the layer, arising from the induced electrostatic field[10] E_x. In order for the current to relax, it is necessary for electrons near the Fermi energy to be scattered from one side of the electron layer to the other, and thus restore the equilibrium population. Since there is little overlap between the two sets of states, this scattering rate should be relatively small, and the resistivity ρ_{yy} for currents in the y direction, at low temperatures in the SDW state, should be reduced considerably below the value in the absence of the magnetic field B_x, and it should similarly be smaller than the values at temperatures above the SDW transition.

By contrast, current in the x direction is carried equally by extended states at both sides of the electron layer; it is not necessary to scatter electrons across the layer to restore equilibrium in this case. We expect that the resistivity ρ_{xx} for currents in the x direction should be higher in the SDW state than in zero magnetic field, or than the resistivity at temperatures above the SDW transition, because electrons near the center of the parabolic well cannot carry a current in the x direction in the SDW state, and the remaining states which contribute to the current are located near the edges where scattering due to the impurities in presumably the strongest.

If dislocations are present in the SDW structure, there will necessarily be states at the Fermi energy in the vicinity of the dislocation which connect the two sides of the electron layer.[3] Such states will clearly increase the relaxation of a current in the y direction, and increase the value of ρ_{yy}. If the distance between dislocations becomes comparable to the period of the SDW, the value of ρ_{yy} will presumably become similar to ρ_{xx}.

We note that for a layer of finite thickness, even in the absence of dislocations the values of both ρ_{xx} and ρ_{yy} should be finite at $T=0$. For thick wells the sheet resistance should essentially be independent of thickness, for currents in the x direction, since the surface conduction may be supposed to be independent of the layer thickness. On the other hand, the values of ρ_{yy} should decrease rapidly with the thickness of the electron layer, for a SDW with no dislocations. In particular, if one consider a hypothetical situation of a parabolic potential of fixed curvature (i.e., fixed n_0) and unlimited width, then the value of ρ_{yy} might be expected to decrease exponentially with the thickness of the electron layer.

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