# Correlations in two-dimensional electron systems. Magnetic properties

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The ground-state energies of (i) an ideal two-dimensional electron gas, (ii) a quasi-twodimensional electron system resembling electrons trapped on a liquid-helium surface, (iii) a quasitwo-dimensional electron system resembling inversion layers of the Si(100)-SiO<sub>2</sub> system, and (iv) an ideal three-dimensional electron gas are obtained by numerically evaluating the sum of "ring diagram" contributions to the correlation energies for all magnetizations and a wide range of electron densities. The transition from nonmagnetic to ferromagnetic state is abrupt in (i) and (ii) and gradual in (iii) and (iv). It is argued that these transitions may occur in quasi-twodimensional systems without violating the theorems on the nonexistence of long-range order in two dimensions because of the presence of weak long-range forces in such systems.

## I. INTRODUCTION

Electrons placed on the surface of liquid helium and electrons attracted to a silicon-silicon dioxide interface by an electric field are two examples of quasi-twodimensional electron systems. Recent experimental and theoretical work on these systems indicate that an appropriately modified two-dimensional electron-gas model may describe the essential physics of these systems.<sup>1</sup> Properties of the unmodified two-dimensional electron gas are also of interest since they provide a simple standard for comparison.

A particularly appealing aspect of these twodimensional systems is that the electron density can be experimentally varied. As the density is lowered, interactions become relatively important, and one might expect to see the effects of these interactions in the form of new states of the system and phase transitions between these states. It is difficult to calculate what electronic configuration will be stable at a given density, and a great variety of states is conceivable. For example, it has been suggested that electrons at the Si-SiO<sub>2</sub> interface [metal-oxide-semiconductor field-effect transistor (MOSFET)] may be localized in the sense of Anderson or Wigner,<sup>1</sup> or that the electrons form a spin-density wave, a charge-density wave, or a more complicated ordering.<sup>2</sup> The primary purpose of this paper is to present a detailed investigation of the stability of the paramagnetic and ferromagnetic electron ordering in two-dimensional and quasitwo-dimensional systems.<sup>3</sup>

The ferromagnetic state is investigated in part because we believe that ferromagnetic order is a real possibility for some two-dimensional systems. Another reason for considering ferromagnetism lies in the relative simplicity of the problem which allows us to perform better calculations with fewer *ad hoc* parameters. Because we have not investigated all possible electronic configurations, we cannot honestly insist that the electrons will ferromagnetically order if our calculations so indicate. We can, however, be assured that the paramagnetic state is unstable if the ferromagnetic state has lower energy.

Of course, our calculations are not exact and some approximations are unavoidable. A particularly difficult problem is associated with the question of long-range order. Our calculations do not consider the possibility of ferromagnetic order over short distances with long-range disorder. There are, in fact, some important theorems<sup>4-8</sup> which would appear to rule out the existence of long-range order in simple twodimensional systems. We will show, however, that these theorems do not apply in real systems which have long-range interactions and asymmetries.

Our conclusion is that magnetic order is possible in two-dimensional electronic systems, and this order may well be observable at presently attainable electron densities. A complimentary approach to the MOSFET system has been taken by Falicov and Kelly<sup>2</sup> where Fermi-surface geometry was considered in greater detail but many-body effects were parametrized into an effective Hartree-Fock theory. Our calculation provides a quantitative estimate of the parameters which should appear in such a theory.

In Sec. II, we give arguments to show how the exiistence of long-range order in two dimensions can come about via weak but long-range interparticle interactions. In Sec. III, we consider in detail the calculations of the ground-state energy of the quasidimensional system. This is further divided into subsections

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in order to discuss (a) an ideal two-dimensional system; (b) a quasi-two-dimensional system which resembles electrons on liquid helium; (c) the Si(100)-SiO<sub>2</sub> system, and (d) an ideal three-dimensional system. The last one is of interest as an interesting system to compare the results of the quasi-two-dimensional systems. In Sec. IV, we summarize our results.

#### **II. LONG-RANGE ORDER IN TWO DIMENSIONS**

Before proceeding to calculations of the relative stability of ferromagnetism, it is important to consider in what sense ferromagnetism may exist in two dimensions. Theorems of Mermin and Wagner,<sup>4</sup> Hamilton,<sup>7</sup> and Walker and Ruijgrok<sup>8</sup> suggest that there cannot be long-range order. Of course it is still possible that some phase transition could exist even for these systems where the theorems are applicable. More importantly, the theorems are based on some restrictive assumptions which are often invalid in real systems. For example, these theorems require that forces be short ranged and isotropic in at least two dimensions. Real electrons exhibit weak but long-range dipoledipole interactions which are not insignificant. For example, these forces give rise to the distinction between "external" (H) and "internal" ( $B = H + 4\pi M$ ) magnetic fields. If the approximation of replacing Hby B and ignoring dipole-dipole interaction is made and applied to the Mermin-Wagner arguments, one can no longer exclude the possibility of long-range ferromagnetic order. (That such a replacement of H by B in the theory of electron gas occurs in principle has recently been demonstrated by Holstein, Norton and Pincus.)<sup>9</sup> One can, however, suggest that the transition temperature should be decreased by a factor involving the logarithm of the ratio of the exchange interaction to the dipole-dipole interaction. Another argument against ferromagnetic order in two dimensions is that the calculated number of spin waves at any nonzero temperature is infinite. However, if there is any anisotropy in the system due to spin-orbit forces, the spin-wave energy no longer vanishes for very long wavelengths and this divergence disappears. Dipoledipole forces will also change the long wavelength spin-wave dispersion so that the number of spin waves is finite.

Here we will give a simple classical derivation of this result for a system of spins on a square lattice interacting via the usual Heisenberg exchange along with weak dipolar interactions

$$H_{\text{spins}} = -J \sum_{\langle ij \rangle} \vec{\mathbf{S}}_{i} \cdot \vec{\mathbf{S}}_{j} + D$$
$$\times \sum_{\langle ij \rangle} [\vec{\mathbf{S}}_{i} \cdot \vec{\mathbf{S}}_{j} - 3(\vec{\mathbf{S}}_{i} \cdot \vec{\mathbf{n}}_{ij})(\vec{\mathbf{S}}_{j} \cdot \vec{\mathbf{n}}_{ij})] , \qquad (1)$$

where  $\overline{n}_{ij}$  is the unit vector along the line joining the sites *i* and *j*. Assume J >> D so that the ground state

corresponds to all spins up.

The classical equation of motion for spin  $\vec{S}_i$  is

$$\frac{d\,\vec{S}_{\,\prime}}{dt} = \vec{B}_{\rm eff} \times \vec{S}_{\,\prime} \quad . \tag{2}$$

Assuming the x-z plane to be the plane in which our two-dimensional (2-D) array of spins lie, for the square-lattice geometry, we have for the motion of  $\vec{S}_{1,2}$ 

$$\vec{B}_{eff} = (J - D) \left( \vec{S}_2 + \vec{S}_3 + \vec{S}_4 + \vec{S}_5 \right) + 3D \left[ \hat{z} \left( \vec{S}_2 \cdot \hat{z} + \vec{S}_4 \cdot \hat{z} \right) + \hat{x} \left( \vec{S}_3 \cdot \hat{x} + \vec{S}_5 \cdot \hat{x} \right) \right] ; \quad (3)$$

for the case under consideration,

$$S_{n}^{z} \cong S_{z_{0}} = S, \quad S_{n}^{x} \simeq u e^{i(\vec{k} \cdot \vec{n} - \omega t)} ,$$

$$S_{n}^{y} \simeq v e^{i(\vec{k} \cdot \vec{n} - \omega t)} , \qquad (4)$$

where  $u, v \ll S$ . Let

$$A = -2S(J - D), \quad B = 6DS$$
 (5)

Then, from (2)–(5) we obtain for small k,

$$\omega^{2} = A^{2}(\frac{1}{4}k^{4}) + AB(\frac{1}{2}k^{2})[1 + (\frac{1}{2}k_{x}^{2})] + B^{2}(\frac{1}{2}k_{x}^{2}) \quad .$$
(6)

Thus, for small k,  $\omega \approx k$  instead of  $k^2$ , and the number of spin waves is finite.

One might also argue that surface imperfections should destroy long-range order in some twodimensional systems. In fact, Imry and Ma<sup>10</sup> and Sham and Patton<sup>11</sup> have shown for systems with a continuous (rotational) symmetry and short-range forces that an arbitrarily small random magnetic field will destroy the long-range order. Again, we argue that these results must be treated with caution in real systems with anisotropy and residual long-range forces.

In our view, the question of the existence of twodimensional ferromagnetism (or any such magnetic order) in real itinerant electron systems is a two-part problem. There is the question at gross level of the relative energetics of ferromagnetic and paramagnetic orders and the delicate question of existence of longrange order in two-dimensional systems. In considering these two problems, one may need to perform different but seemingly inconsistent model calculations. For example, possible long-range order in two dimensions is related to the questions of rotational symmetry and long-range forces. Anisotropy fields and dipole-dipole interactions are present in real systems and these effects cannot be ignored since they may stabilize the ferromagnetism. On the other hand, any quantitative calculation of the relative energy of itinerant electron ferromagnetic and paramagnetic states is dominated by a comparison of kinetic and Coulomb energies. The very small dipole-dipole and anisotropy energies would appear to be *insignificantly* small in these calculations and as such they are ignored. Strictly speaking, then, when our calculations indicate ferromagnetism, we are really implying that the Coulomb interactions with exchange effects lead to significant short-range ferromagnetic order, and at sufficiently low temperatures the weak long-range forces should change this short-range ferromagnetic order into a real two-dimensional ferromagnetic one.

One could argue that the forces which allow longrange order in two dimensions are so weak that ferromagnetism might occur only at very low temperatures. However, these weak forces can become effectively strong when there is significant short-range order so that one can consider the interaction of "blocks" of spins rather than individual electrons. When the "blocks" become large the dipole-dipole and anisotropy interactions become more important and may lead to ferromagnetic order, at a relatively high temperature.

## **III. STABILITY OF FERROMAGNETISM**

The method we use to estimate relative ferromagnetic stability in two dimensions is based on the numerical calculations of the sum of ring diagrams. At high densities these ring diagrams give the correct high-density Gell-Mann-Brueckner series expansion<sup>12</sup> of the ground-state energy. At low densities, Iwata<sup>13</sup> has shown that in three dimensions these same diagrams yield a good low-density expansion of the ground-state energy. We, thus, have some confidence that an exact evaluation of the ring-diagram contribution to the ground-state energy of an electron gas may be a good interpolation formula for the entire range of electron densities, and the evaluation of these energies can give good estimates concerning the stability of ferromagnetism. The results presented here are, in part, an extension of previous works where the first few terms in the high-density expansion of the ground-state energy of the two-dimensional electron gas were presented,<sup>14</sup> and the ferromagnetic stability in the two-dimensional electron gas was investigated in the Hartree-Fock approximation.<sup>3</sup>

There have been other calculations of the stability of ferromagnetism related to the ring-diagram approximation,<sup>15-18</sup> but in three dimensions. These earlier results do not treat the two-dimensional case as we do. Jonson<sup>19</sup> has only recently published such calculations only for the paramagnetic case for two- and quasitwo-dimensional systems. In addition, we have obtained the pair correlation function at zero separation from the calculated ground-state energy. The correlation function reveals a weakness in the ring-diagram approximation at low densities.

The ring-diagram approximation to the ground-state energy of the quasi-two-dimensional electron gas depends on the electron density and magnetization. The density is specified in terms of the dimensionless quantity  $r_s$ \* given by

$$r_s^* = (2/n_v)^{1/2} (k_F a_0^*)^{-1}$$
, (7)

where  $k_F$  is the Fermi wave vector, and  $n_v$  is the band degeneracy. For electrons on the surface of helium, and the simple electron gas  $n_v = 1$ , but for the MOS-FET there is more than one piece of Fermi surface and  $n_v$  may be four or six depending on crystallographic orientation. The quantity  $a_0^*$  is the effective Bohr radius of the system

$$a_0^* = (\bar{\kappa}/m^*)a_0$$
, (8)

with  $\overline{\kappa}$  being an average dielectric constant. For the MOSFET  $\overline{\kappa}$  is the average of the SiO<sub>2</sub> and Si dielectric constants. The effective mass  $m^*$  is measured in units of the free-electron mass. The magnetization of the system is given as

$$\zeta = (n_1 - n_1) / (n_1 + n_1) \quad , \tag{9}$$

where  $n_1(n_1)$  specifies the density of spin-up (down) electrons.

The leading order term in the high-density expansion of the electron-gas energy is simply the kinetic energy of the noninteracting electrons

$$E_{\rm kin} = (1+\zeta^2)/n_{\rm y}r_{\rm s}^{*2} , \qquad (10)$$

where all energies are expressed in renormalized Rydberg units (=13.6 eV ×  $m^*/\kappa^2$ ).

The next term in the energy expansion is the exchange energy which can be written

$$E_{\rm ex} = \left(\frac{2}{n_{\rm v}}\right)^{1/2} \frac{\bar{\kappa}/\kappa}{4\pi^2 r_{\rm s}^*} \sum_{\sigma} \int d^2k \ d^2k' \ V(\vec{k} - \vec{k}') \times f_{\sigma}(k) f_{\sigma}(k') \quad . \tag{11}$$

All wave vectors here and in subsequent formulas are scaled by the Fermi momentum  $k_F$ . Here  $f_{\sigma}(k)$  is the zero-temperature Fermi function for the spin  $\sigma$  electron with wave vector k and  $\kappa$  is the dielectric constant of the material in which the electrons reside. The quantity V(q) is the Fourier transform of an effective electron-electron interaction. In general, V(q) diverges with 1/|q| as q goes to zero, and for the simple two-dimensional electron gas

$$V(q) = |\vec{q}|^{-1} .$$
 (12a)

More generally, V(q) depends on the material and its form is given here, which takes into account the finite extent of the electron wave function and image effects<sup>1,19</sup>

$$V(q) = q^{-1}(\bar{\kappa}/\kappa_{\rm sc})F(q) \quad , \tag{12b}$$

where<sup>1,19</sup>

$$F(q) = \frac{3}{8}(1+q/b)^{-1} + \frac{3}{8}(1+q/b)^{-2} + \frac{1}{4}(1+q/b)^{-3} + \delta(1+q/b)^{-6} , \qquad (12c)$$

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with

$$\delta = (\kappa_{\rm sc} - \kappa_{\rm in}) / (\kappa_{\rm sc} + \kappa_{\rm in})$$
(12d)

arises from the image forces.  $\kappa_{sc}$  and  $\kappa_{in}$  are the dielectric constants of the semiconductor and insulator, respectively. The finite extent of the wave function is parametrized by *b* and it is chosen to be

$$b/k_F = [12.2^{1/2} \times n_v^{3/2}(m_3^*/m^*) \times (\bar{\kappa}/\kappa_{\rm sc})r_s^*(\frac{11}{32} + N_{\rm dep}/N)]^{1/3} .$$
(12e)

 $N_{dep}$  is the number of electrons in the depletion layer and  $m_3^*$  is the effective mass of the electron in the transverse direction. For He,  $N_{dep} = 0$ .

The next contribution to the energy  $E_2$  comes from the lowest-order ring diagram. In two dimensions this term is not divergent as it is in three dimensions,

$$E_{2}^{(ex)} = \frac{(\bar{\kappa}/\kappa)^{2} n_{v}}{(2\pi)^{3}}$$

$$\times \sum_{\sigma} \int d^{2}k \ d^{2}k' \ d^{2}q \ f_{\sigma}(k) f_{\sigma}(k')$$

$$\times [1 - f_{\sigma}(|\vec{k} + \vec{q}'|)][|1 - f_{\sigma}(|\vec{k}' + \vec{q}|)]$$

$$\times \frac{V(q) V(|\vec{q} + \vec{k} + \vec{k}'|)}{q^{2} + \vec{q} \cdot (\vec{k} + \vec{k}')} \qquad (13)$$
The last contribution to the total approx  $E$  appear

The last contribution to the total energy  $E_r$  comes from the sum of all higher-order ring diagrams,

$$E_r = \frac{1}{2\pi^2 r_s^{*2} n_v^2} \int_{-\infty}^{\infty} du \int d^2 q |q| [\ln(1+x) - x] , \qquad (14)$$

where

$$x = [(\bar{\kappa}/\kappa)r_{3}^{*}/\sqrt{8}\pi]n_{v}^{3/2}V(q)[Q_{q1}(u) + Q_{q1}(u)]$$
(15)

and

$$Q_{q\sigma}(u) = \int d^2k \int_{-\infty}^{\infty} dt f_{\sigma}(k) [1 - f_{\sigma}(|\vec{\mathbf{k}} + \vec{\mathbf{q}}|)] \\ \times \exp[ituq - |t|(q^2/2 + \vec{\mathbf{q}} \cdot \vec{\mathbf{k}})] \quad .$$
(16)

The calculation of the energy and its magnetization dependence consist of numerically evaluating the sum

$$E = E_{\rm kin} + E_{\rm ex} + E_2^{(\rm ex)} + E_{\rm ring}$$
, (17)

for various systems. We have omitted here a contribution to the energy arising from the finite extent of the electronic wave function which in the scheme employed here does not depend on  $\zeta$ . We shall discuss these separately now.

#### A. Ideal two-dimensional system

In an ideal two-dimensional system, the system parameters are very simple. All the dielectric constants and the effective masses are unity. There is no valley degeneracy  $(n_v = 1)$ . The energy is measured in Rydbergs and the dimensionless parameter  $r_s$  \* is denoted by  $r_s$  and is given by Eq. (7) with  $a_0$  \* replaced by  $a_0$ . Moreover, V(q) is given by (12a). Then  $E_2^{(ex)}$  becomes independent of magnetization and density and is a mere constant.<sup>14</sup> The dependences of  $Q_q(u) = Q_{q\sigma}(u)$  with  $\zeta = 0$  on q for various values of u are shown in Fig. 1. Clearly the sharp cutoff approximation used in the high-density approximation<sup>14</sup>  $Q_{a}(u) \simeq 2\pi R(u)$  independent of q, can lead to significant errors and, in fact, we find substantially different results for calculations performed with and without this approximation.

In Fig. 2, the ground-state energy of the twodimensional paramagnetic and ferromagnetic states are displayed. The insert in the lower right shows difference in these energies. Thus, according to this calculation, the transition to the ferromagnetic state occurs abruptly at  $r_s \approx 5.4$ , which is a considerably larger value than the result obtained in Hartree-Fock approximation  $(r_s^{\text{HF}} \approx 2)$  or by making the highdensity approximation  $(r_s^{\text{GB}} \approx 2.3).^{14}$ 

By investigating the energy of partially magnetized states, we have found that these states are *never* stable. Thus, the transition to the ferromagnetic state occurs abruptly at  $r_s \simeq 5.4$  in an ideal two-dimensional system.

## B. Quasi-two-dimensional system – Electrons on liquid helium

This model is similar to the ideal system in that the dielectric constants  $\kappa_{in} \approx 1.053$ ,  $\kappa_{sc} \approx 1$ , and effective masses are unity and there is no valley degeneracy. The only new effect here is the finite extent of the



FIG. 1. Function  $Q_q(u)$  in two dimensions as a function of q with u held constant. Individual curves are labeled by the value of u. These curves should be compared with the sharp cutoff approximation  $Q_q(u) \simeq 2\pi R(u)$ .



FIG. 2. Two-dimensional electron gas energy per particle as a function of the density parameter  $r_s$ . Curves labeled Fand P correspond to the energies of the saturated ferromagnetic and the paramagentic states. The dotted curve on the lower right is the energy difference between the paramagnetic and ferromagnetic states ( $\Delta E$ ), and the vertical scale for this curve is on the right-hand side.

wave function introduced via the parameter b which is taken here to be given by Eq. (12e) with  $N_{dep} \equiv 0$ . The energies are again measured in Rydbergs and the dimensionless parameter is  $r_s$  as in A. In a sense, this calculation is the same as the one described in A but with the only new feature of the "finite-thickness" effect incorporated here. Our numerical results are similar to those of A: abrupt transition to the ferromagnetic state ( $\zeta = 1$ ) at  $r_s \simeq 11$ . The effect of finite thickness is thus to move the transition to a lower density.

 $E_2^{(ex)}$  now depends on  $r_s$  and  $\zeta$  but the numerical calculations are not accurate enough to estimate its effect.

# C. Quasi-two-dimensional system-Si(100)-SiO<sub>2</sub> system

We have done the numerical calculation for two representative values<sup>1,19</sup> of  $N_{dep}$ ; 7.6 × 10<sup>10</sup> and 7.6 × 10<sup>11</sup>/cm<sup>2</sup>. The parameters used here are

$$m_3^* = 0.9, \quad m^* = 0.19, \quad n_v = 2,$$
  
 $\kappa_{sc} = 11.8, \quad \kappa_{in} = 3.8;$ 
 $(18)$   
 $\mathfrak{R}^* \to 42.5 \text{ meV}; \quad a_0^* = 41a_0.$ 



FIG. 3. Magnetization dependence of the energy per particle of the quasi- 2-D electron gas system in Si(100)-SiO<sub>2</sub>. Curves are labeled by values of  $r_s$  and are for  $N_{dep} = 7.6 \times 10^{10}/\text{cm}^2$ . Note the occurrence of possible partial magnetization for  $r_s$  near 12 and the fully magnetized state occurs only after  $r_s$  exceeds 13.

Here we use the dimensionless parameter  $r_s$ <sup>\*</sup>. The calculation of the total energy as a function of  $r_s$  \* for  $\zeta = 0$  with  $N_{dep} = 7.6 \times 10^{10} / \text{cm}^2$  has been done by Jonson<sup>19</sup> without the second-order exchange term and our numerical results agree with his. In Fig. 3, we have displayed a calculation of the energy as a function of  $\zeta$ for representative values of r, \* for  $N_{dep} = 7.6 \times 10^{10} / \text{cm}^2$ . In contrast to cases A and B, we find the transition to be gradual. For  $N > 4.6 \times 10^{10} / \text{cm}^2$  we have  $\zeta = 0$  state;  $3.99 \times 10^{10}$  $< N < 4.6 \times 10^{10}$ /cm<sup>2</sup> states with  $0 < \zeta < 1$ have a minima and for  $N < 3.99 \times 10^{10}/\text{cm}^2$ ,  $\zeta = 1$  is the ground state. For  $N_{dep} = 7.6 \times 10^{11} / \text{cm}^2$ , similar results are obtained but states with  $0 < \zeta < 1$  now occur for  $5.6 \times 10^{10} < N < 8.3 \times 10^{10} / \text{cm}^2$  and  $\zeta = 1$  for  $N < 5.6 \times 10^{10}$ /cm<sup>2</sup>. These values of electron densities in the inversion layer are in the experimental range.

## D. Ideal three-dimensional system

For the sake of completeness and for providing an interesting comparison with the cases considered above, we have also calculated the magnetic properties of an ideal three-dimensional (3-D) electron gas. It may be pointed out that previous calculations<sup>15-18</sup> are not as complete as those presented here. Our results are given in Fig. 4. Misawa's<sup>15</sup> high-density approxi-



FIG. 4. Magnetization dependence of the energy per particle of the three-dimensional electron gas. Curves are labeled by values of  $r_s$ . Note that the instability for partial magnetization occurs for  $r_s$  near 14, but the fully magnetized state occurs only after  $r_s$  exceeds 17.

mation was incorrect and we find in a similar approximation that there is an abrupt transition to ferromagnetic state for  $r_s > 6.1$ . In Refs. 16–18, the value of  $r_s$ , where the transition may occur, was only estimated but not actually calculated. Our calculations indicate that there is a narrow range of densities corresponding to  $14 < r_s < 17.3$  where  $0 < \zeta < 1$  is probably stable and for  $r_s > 17.3$ , states with  $\zeta = 1$  and for  $r_s < 14$  states with  $\zeta = 0$  are the ground states. This is similar to case (C) above.

#### **IV. SUMMARY**

The major point of this work is that ferromagnetism may be observable in quasi-two-dimensional systems. We must, of course, acknowledge the possibility of large errors in our (and any other) approximate calculation. This makes the conclusions speculative.

The discussion of the stability of various possible types of states considered here and elsewhere<sup>2</sup> must be considered speculative since all these calculations are approximate. In Ref. 2., only HF approximation was used which takes into account parallel spin correlations among the electrons. One knows from the work in 3-D systems, inclusion of correlation effects destroys the phase transitions deduced in the HF scheme. On the other hand, our calculation takes into account some of the correlation contributions beyond HF, but it is not variational in character. It should be stressed that our calculation has the virtue of being exact for asymptotically high<sup>12</sup> and low<sup>13</sup> densities. A variational calculation of the ground-state energy is difficult and none exist for the 2-D electron system. In 3-D, a Jastrow-type trial solution has been tried and tentative conclusions similar to what we have reached (Item 4 in Table I) are obtained. This is because, here again, the expectation value of the Hamiltonian in the trial state cannot be calculated exactly. It is interesting to note that Gaskell showed that the Gell-Mann-Brueckner result<sup>12</sup> may be obtained by considering a simple form for the Jastrow trial state. (This wave function simulated the collective plasmon oscillation, which in the GB scheme is properly accounted for.) A fully reliable answer can only be obtained when a variational scheme is successfully incorporated in exploring the various ground states of this or any other system. Until then, all these results (this

TABLE I. Regions of magnetic stability of the electron systems.

System	Paramagnetism $(\chi = 0)$	Unsaturated ferromagnetism $(0 < \zeta < 1)$	Ferromagnetism (ζ = 1)
Ideal two dimensions	$r_{s} < 5.4$	unstable	$r_{s} > 5.4$
Quasi-two-dimensions			
$(e^{-} \text{ on liquid He})$	$r_{s} < 11$	unstable	$r_{s} > 11$
Quasi-two-			$r_{s}^{*} > 13$
dimensions inversion $N_{dep} = 7.6 \times 10^{10} / \text{cm}^2$	$r_s^* < 12(N > 4.6 \times 10^{10} / \text{cm}^2)$	$12 < r_s^* < 13$	$(N < 3.99 \times 10^{10}/\text{cm}^2)$
layer (Si(100)-SiO <sub>2</sub>			$r_{s}^{*} > 11$
System) $N_{dep} = 7.6 \times 10^{11} / cm^2$	$r_{\rm v}^* < 9(N > 8.3 \times 10^{10} / {\rm cm}^2)$	$9 < r_s^* < 11$	$(N < 5.6 \times 10^{10} / \text{cm}^2)$
Ideal three		-	
dimensions	$r_{s} < 14$	$14 < r_s < 17.3$	$r_{s} > 17.3$

paper, as well as Ref. 2.) have to be considered as speculative, at best. The pair-correlation function for the ideal system can be calculated by differentiating formally the total energy with respect to the Coulomb potential, V(q) and from a ground-state energy calculation of Sec. III A, the pair correlation function at zero separation was calculated. Our results are found to be unphysical for  $r_{\chi} \ge 2.4$  and they point to a weakness in the ring-diagram approximation. How serious this weakness is in terms of errors in the ground-state energy is not clear from this calculation. In three dimensions, a similar calculation of the pair correlation function at zero separation was found to become negative for r > 2.6.

The results of our ground-state energy calculation are summarized in Table I. It appears from this that

- <sup>1</sup>Proceeding of an International Conference on the Electron Properties of Quasi-Two-Dimensional Systems (to be published in Surf. Sci.); B. Vinter, Phys. Rev. B <u>13</u>, 4447 (1976).
- <sup>2</sup>M. J. Kelly and L. M. Falicov, Phys. Rev. Lett. <u>37</u>, 1021 (1976); M. J. Kelly and L. M. Falicov, Phys. Rev. B <u>15</u>, 1974 and 1983 (1977).
- <sup>3</sup>A. K. Rajagopal, Solid State Commun. <u>21</u>, 483 (1977); a brief account was presented in ICM 76 (Amsterdam 1976), its proceedings in Physica (Utr.) B <u>86–88</u>, 373 (1977).
- <sup>4</sup>N. D. Mermin and H. Wagner, Phys. Rev. Lett. <u>17</u>, 1133 (1966).
- <sup>5</sup>P. Hohenberg, Phys. Rev. <u>158</u>, 383 (1967).
- <sup>6</sup>N. D. Mermin, Phys. Rev. <u>176</u>, 250 (1968).
- <sup>7</sup>D. C. Hamilton, Phys. Rev. <u>157</u>, 427 (1967).
- <sup>8</sup>M. B. Walker and Th. W. Ruijgrok, Phys. Rev. <u>171</u>, 513

ferromagnetism may be possible in the Si(100)- $SiO_2$  system in a realistic density region of the inversion layer.

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(1968).

- <sup>9</sup>T. Holstein, R. E. Norton, and P. Pincus, Phys. Rev. B <u>8</u>, 2649 (1973).
- <sup>10</sup>Y. Imry and S. K. Ma, Phys. Rev. Lett. <u>35</u>, 1399 (1975).
- <sup>11</sup>L. J. Sham and B. R. Patton, Phys. Rev. B <u>13</u>, 3151 (1976).
- <sup>12</sup>M. Gell-Mann and K. A. Brueckner, Phys. Rev. <u>106</u>, 364 (1957).
- <sup>13</sup>G. Iwata, Prog. Theor. Phys. <u>24</u>, 1118 (1960).
- <sup>14</sup>A. K. Rajagopal and J. C. Kimball, Phys. Rev. B <u>15</u>, 2819 (1977).
- <sup>15</sup>S. Misawa, Phys. Rev. <u>140</u>, A1645 (1965).
- <sup>16</sup>L. Hedin, Phys. Rev. <u>139</u>, A796 (1965).
- <sup>17</sup>U. von Barth and L. Hedin, J. Phys. C 5, 1629 (1972).
- <sup>18</sup>J. Lam, Phys. Konden. Mater. <u>15</u>, 46 (1972).
- <sup>19</sup>M. Jonson, J. Phys. C <u>9</u>, 3055 (1976).

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