

## Charge-density waves in two- and three-dimensional jellium

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The stability of the electron gas in jellium against the formation of charge-density waves is studied using the density-functional formalism. Charge-density waves occur in three-dimensional jellium for  $r_s > 26$  and in two dimensions for  $r_s > 17$  in our approximation. The theory is applied to two-dimensional electron gases on liquid-helium surfaces and in semiconductors.

### I. INTRODUCTION

The nature of the ground state of electrons in solids has long been investigated using the "jellium" model in which the electrons move in a rigid uniform positive background. At high electron density  $n$ , (i.e., small  $r_s$ , where  $\frac{4}{3}\pi r_s^3 = 1/n$ ) the ground state is the usual spatially uniform paramagnetic electron gas which shares many properties with electrons in metals. These properties are dominated by the large zero-point kinetic energy arising from Pauli principle. At low densities the electron-electron interactions become relatively more important, and we can expect the spatial density to become *nonuniform* to minimize the energy by keeping electrons out of one another's way. This was first pointed out by Wigner<sup>1</sup> who hypothesized a crystallized phase of electrons<sup>2,3</sup> at very large  $r_s$ .

It is natural to inquire about the nature of the onset of Wigner crystallization and, in particular, whether there are precursors to the crystallized phase: that is, inhomogeneities driven by the Coulomb repulsion of electrons. Overhauser<sup>4</sup> considered such effects for a model different from jellium. These are called charge-density waves (CDW's). In Overhauser's model the background is not rigid, but completely deformable (as the ions in alkali metals might be). If the electron gas is treated in the Hartree-Fock approximation it is unstable against CDW's at any density, though correlation probably moves the instability to low density.<sup>5</sup>

In this paper we inquire when CDW instabilities occur in jellium and how they set in. It is clear that such instabilities must occur at some density because the Wigner crystal can be regarded as a CDW state in extreme form. This point has caused some confusion in the past.<sup>6</sup>

Our technique is to use the density-functional method.<sup>7,8</sup> This takes into account exchange and

correlation in an approximate way (the local approximation) and is uniquely suited to calculate energy differences between uniform and nonuniform states. In Sec. II we discuss the method and outline how we apply it to our problem.

Our motivation in this work is twofold. First, we are interested in the structure of the theory and how it compares to previous theories of the three-dimensional Wigner crystal and charge-density waves. These points are discussed in Sec. III. We also briefly discuss possible magnetic states such as spin-density waves and how corrections to the local approximation might modify our result. Second, we are interested in physical systems that approximate jellium and which might show CDW instabilities of the sort we discussed here. The systems we are aware of are all effectively two dimensional. Section IV outlines our results in two dimensions applied to cases of experimental interest, namely, inversion layers and heterostructures in semiconductors and surface bound electrons on helium. Section V gives a brief summary.

We should point out that all the examples of CDW's yet observed occur in systems very unlike jellium such as transition-metal dichalcogenides and certain chain compounds.<sup>9</sup> It is widely believed that CDW's in these materials are driven by peculiar features of the Fermi surface and/or a strong electron-phonon interaction.<sup>6</sup> We take no account of such effects in this paper.

### II. FORMULATION OF THE THEORY

We seek to find the spatial nature of the ground state of  $n_0$  electrons per unit volume in a rigid positive background. We compare the energy of the uniform state with certain inhomogeneous states where

the density takes the form

$$n(\vec{r}) = n_0 + n_1 \cos \vec{q} \cdot \vec{r} . \quad (1)$$

This is a CDW of wave vector  $\vec{q}$  and amplitude  $n_1$ .

We need the ground-state energy for various values of  $n_0$  as a function of the deformation. The

$$E(n(r)) = T + \frac{1}{2} \int \frac{[n(\vec{r}_1) - n_0][n(\vec{r}_2) - n_0]}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_1 d\vec{r}_2 + \int n(\vec{r}) \epsilon_{xc}(n(\vec{r})) d\vec{r} . \quad (2)$$

In this expression  $T$  is the kinetic energy of a system of noninteracting electrons which are subjected to sufficient external potentials to acquire the density  $n(\vec{r})$  and  $\epsilon_{xc}(n)$  is the exchange and correlation energy per particle of a uniform electron gas of density  $n$ . This expression rests on firm theoretical foundations<sup>7,8</sup> for systems which are nearly homogeneous (which is our interest here) and has been tested in a wide variety of physical situations.

For low density there are some problems connected with the last term of Eq. (2) which uses the "local approximation" for exchange and correlation, that is, the integrand depends only on  $n(r)$ . The local approximation works very well at high densities<sup>8</sup> but its validity at low densities has not been tested. As we will see, we treat  $\epsilon_{xc}$  in such a way that the theory is correct for the extreme low-density limit (the Wigner crystal). We will discuss this point further below.

There are two ways to apply the theory to our problem depending on how the CDW instabilities occur. We know that for  $n_0$  large there is no deformation ( $n_1 = 0$ ). At some critical value,  $n_0 = n_c$ , deformation sets in and it may occur continuously ( $n_1$  small for  $n_0 = n_c - \delta$ , a second-order transition) or discontinuously ( $n_1$  finite for  $n_0 = n_c - \delta$ , a first-order transition). We consider these two possibilities separately.

(i) If a second-order transition should happen to occur our approach can be the classic method of Landau and Lifshitz.<sup>10</sup> We note that  $n_1$  be considered to be the order parameter of our transition. Clearly,  $\epsilon(n)$  is even in  $n_1$  so that  $\delta\epsilon/\delta n_1 = 0$  for  $n_1 = 0$ . If this extremum of the energy is to be stable  $\delta^2\epsilon/\delta n_1^2 > 0$ ; if  $\delta^2\epsilon/\delta n_1^2 < 0$  the system will simultaneously distort and a CDW will set it. Thus, the signal of a continuous transition is the vanishing of  $\delta^2\epsilon/\delta n_1^2$ . Now from Eqs. (1) and (2) and a brief calculation the transition will occur if

$$0 = \frac{1}{\Omega} \frac{\delta^2\epsilon}{\delta n_1^2} \Big|_{n_1=0} = \frac{1}{\Omega} \frac{\delta T}{\delta n_1^2} + v(q) + \frac{d^2(n\epsilon_{xc})}{dn^2} \Big|_{n_0} , \quad (3)$$

$$v(q) = \int d\vec{r} e^{-i\vec{q}\cdot\vec{r}/r} = \begin{cases} 4\pi/q^2 , \\ 2\pi/q , \end{cases} \quad (4)$$

for three and two dimensions, respectively. Here  $\Omega$

function required is provided very conveniently by the density-functional theory of Hohenberg and Kohn<sup>7</sup> and by Kohn and Sham.<sup>8</sup> The theory tells us that the ground-state energy can be written to a good approximation as follows (atomic units are used throughout this paper):

is the volume (or area) of the system. The right-hand side of Eq. (4) is simply related to the dielectric function; Eq. (4) corresponds to setting  $\epsilon - 1 = 0$ .

The first term in Eq. (3) is well known in electron-gas theory: it is the inverse of the density-response function,  $\chi_0$ , of the free-electron gas. This identification follows at once if we recall that the change in energy for the free-electron gas when distorted is

$$\delta E = n_1^2 / 2\chi_0(q) , \quad (5)$$

$$\chi_0(q) = \frac{\sum [f(k) - f(k+q)]}{\epsilon_0(k) - \epsilon_0(k+q)} . \quad (6)$$

Here  $f$  is the (zero-temperature) Fermi function and  $\epsilon_0$  the free-electron energy. The function  $\chi_0$  is evaluated in many standard references in two<sup>11</sup> and three<sup>12</sup> dimensions.

Thus we will have a second-order transition if

$$\frac{1}{\chi_0} = - \left[ \frac{d^2(n\epsilon_{xc})}{dn^2} + v(q) \right] . \quad (7)$$

This is a form of the Chan-Heine criterion<sup>6</sup> for a charge-density wave. Since  $\chi_0$  is positive Eq. (7) is satisfied only if the negative exchange-correlation potential is larger than  $v(q)$ . The authors of Ref. 6 point out that this is unlikely at metallic densities, but it is not at all impossible in principle, as we will see.

(ii) If a first-order transition occurs, a more difficult calculation must be performed. In this case there are two separate local minima in the energy, at  $n_1 \approx 0$  and  $n_1$  finite. At the transition the value of the energy will be the same for both. We are led to evaluate  $E(n)$  for various values of  $n_1$  and  $q$ . This is done using the Kohn-Sham method.<sup>8</sup> We posit a symmetry-breaking potential  $\phi = \phi_1 \cos(qz)$  and solve the associated one-dimensional band-structure problem. If  $\psi$  are the wave functions and  $\eta(k)$  the corresponding energies

$$n(r) = \sum |\psi|^2 , \quad (8)$$

$$T = \sum \eta(k) - \int \phi n d\vec{r} . \quad (9)$$

By varying  $\phi_1$  and  $q$  to minimize  $E(n)$  we can locate

the transition. This technique will, of course, find second-order transitions too, if they occur.

There is a missing element in both these techniques, namely, the function  $\epsilon_{xc}(n)$  for  $n$ 's below metallic densities. We expect the densities for which CDW's occur in jellium to be far out of the range of validity of RPA-like perturbation treatments precisely because CDW's in jellium signal the dominance of potential over kinetic energy. The present authors investigated this density range in the course of a study of the Wigner crystal.<sup>3</sup> The essential point to be made is that  $\epsilon_{xc}$  reflects the nature of the correlations of the electrons; i.e., at sufficiently low densities electrons avoid one another and are on the verge of becoming localized. If we wish to describe such a situation with a density-functional theory  $\epsilon_{xc}$  takes a special form because isolated electrons *have no* exchange-correlation energies and also no self-electrostatic energy. We choose  $\epsilon_{xc}$  so that these energies cancel (as they do in Hartree-Fock theory). The remarkable fact is that a local  $\epsilon_{xc}$  can be chosen to cancel the nonlocal Hartree term for a very large class of charge-density profiles.

The forms to choose are in, atomic units (1 a.u. = 2 Ry):

$$\lim_{n \rightarrow \infty} \epsilon_{xc}(n) = \begin{cases} -1.66n^{1/2} \\ -1.09n^{1/3} \end{cases} \quad (10)$$

for two and three dimensions, respectively. As Ref. 3 makes clear these are the best local  $\epsilon_{xc}$ 's as  $n \rightarrow 0$ . Since we will always work at very low densities, we use these limiting forms in our calculations.

### III. RESULTS IN THREE DIMENSIONS

(i) *Dielectric-function method.* It is a simple matter to solve Eq. (7) using the standard form<sup>12</sup> for  $\chi_0$ . The equation is most conveniently rewritten

$$F(x) = 9.72n^{1/3}/(1.47 - x^{-2}) \quad , \quad (11)$$

where

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right| \quad , \quad (12)$$

$$x = q/2k_F \quad , \quad (13)$$

and  $k_F$  is the Fermi wave vector.

For large density there is no solution to Eq. (11), and for small density two solutions; see Fig. 1. The instability occurs when a solution starts to exist. We find this to be at  $r_s = 25.4$  and  $q/2k_F = 0.99$ . Note that  $q \approx 2k_F$  for this transition and that we have a situation reminiscent of Overhauser's<sup>4</sup> Fermi-surface instabilities.

(ii) *First-order transitions.* In our previous work<sup>3</sup> on

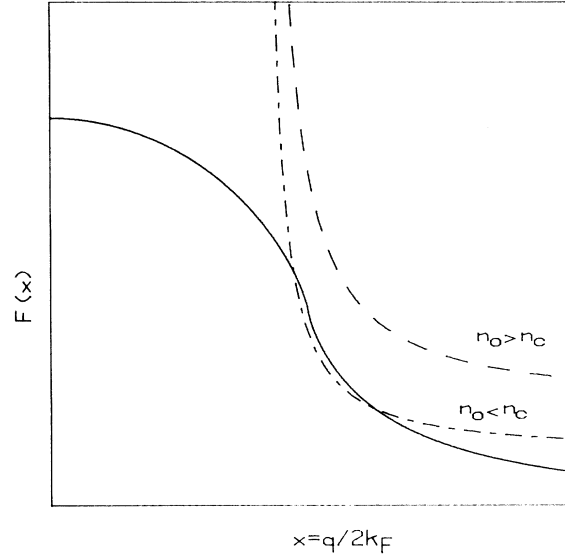


FIG. 1. Graphical solution to Eq. (11). Solid line: Right-hand side (proportional to  $\chi_0$ ). Dashed lines: Left-hand side for  $n_0$  above and below the transition.

the Wigner crystal we found a first-order transition at  $r_s \approx 26$ , but in that work we only investigated crystallization into a close-packed structure. One of our motivations in this paper was to see whether the order of the transition would change if more general symmetries like CDW's were allowed.

We solved numerically for the band structure induced by a self-consistent CDW potential as outlined above. We found a first-order transition once more; however, it occurs at only slightly higher density than the second-order calculation would indicate, and at essentially the same  $q$ ; i.e.,  $r_s \approx 25$  and  $q = (0.99)2k_F$ .

We conclude that the simple calculation using Eq. (7) gives reliable results in this case, even though the phase transition seems to be first order.

(iii) *Magnetic states.* We have not yet considered possible magnetic states of the electron gas. Early work on this subject has been extensively reviewed by Herring,<sup>5</sup> who concludes that while uniform ferromagnetism is unlikely for any density, states of nonuniform magnetization but uniform density (similar to the spin-density waves which are observed in Cr) cannot be ruled out.

We have not included magnetic states in our formalism. We should note that this is not necessarily a defect: The density-functional theory should, in principle, yield the correct spatial state provided the correct  $\epsilon_{xc}$  is inserted. In practice better physical insight is provided by using the *spin*-density-functional formalism which yields the magnetic state as a by-product. We have not used this method because we

have no reliable way to find  $\epsilon_{xc}$  as a function of the densities of spin-up and spin-down electrons at low total density.

Related questions have been investigated recently by Ceperley<sup>13</sup> and Perdew<sup>14</sup> and by Perdew and Datta.<sup>15</sup> Ceperley did a correlated basis-function treatment involving an extensive numerical calculation. He finds a ferromagnetic transition at  $r_s = 26$  and a Wigner crystal for  $r_s > 67$ , in clear disagreement with this work. We believe that Ceperley systematically underestimates the stability of the slightly distorted state because he adopts crystal wave functions appropriate to an extreme low-density limit with a large amount of localization and magnetic order built in (i.e., an insulating state). In our previous work on Wigner crystallization<sup>3</sup> we argued that near the transition the electrons would not be particularly localized even though their density is not uniform and that overlap effects would make treatments such as Ceperley's unreliable except at very low density. In fact, it is possible that the phase Ceperley treats is separate from the one we are concerned with here. That is, there are possibly two phase transitions, one to an inhomogeneous state (perhaps near  $r_s = 26$ ) and another, at lower density (probably signaled by the appearance of magnetic order) to a truly localized state.

Perdew and Datta<sup>15</sup> do dielectric-function calculations similar to ours; however, they use  $\epsilon_{xc}$ 's extracted from Ceperley's work, and allow for magnetic transitions in spin-density-functional formalism. In the local-spin-density approximation they find no disagreement with our results: Their treatment yields a CDW transition around  $r_s = 22$  and no spin-density waves. The only magnetic transition found is the possibility of a uniform ferromagnetic phase for  $22 < r_s < 67$  if certain approximations for a nonlocal  $\epsilon_{xc}$  are used.

Incidentally, it is easy to see why true spin-density waves cannot occur in a theory of the present sort: The analog to Eq. (7) for a spin-density wave is

$$\frac{1}{\chi_0(q)} = - \frac{d^2(n\epsilon_{xc})}{dm^2}, \quad (14)$$

where  $m = n_+ - n_-$  is the amplitude of the spin-density wave [cf. Ref. 6, Eq. (20)]. Since  $\chi_0$  has its maximum at  $q = 0$  the instability sets in at  $q = 0$ , which corresponds to ferromagnetism. The key assumption made in deriving Eq. (14) is the absence of nonlocal ( $q$ -dependent) terms on the right-hand side which differ for spin up and spin down. Since at low densities correlations keep electrons apart most of the time and reduce the spin-dependent exchange terms, the assumption is probably reasonable. The same reasoning implies that the right-hand side of Eq. (11) should be quite small.

(iv) *Nonlocal corrections.* In our view, the weakest

point in our theory is our use of a local density form for  $\epsilon_{xc}$ . The development of corrections to the approximation is the subject of intense current research.<sup>16</sup>

The most commonly used form for such a correction is the gradient approximation which adds to Eq. (2) a term of the form<sup>7</sup>

$$\int g(n) |\nabla n|^2 d^3r. \quad (15)$$

The function  $g(n)$  is known at high densities and attempts have been made to extend its use to metallic densities,<sup>16</sup> with, however, no striking success.

We can only comment on a constraint on the function  $g(n)$  which is implied by the point of view of this paper. If Eqs. (2) and (15) are to describe the transition to an inhomogeneous state and, eventually, Wigner crystallization there is a relationship between  $g(n)$  and  $\epsilon_{xc}(n)$  for small  $n$ . To be specific, in the Wigner crystal electrons are isolated from one another and are well described by a product of independent wave functions. The self-electrostatic-energy term, the self-exchange-correlation term, and the gradient term must *exactly* cancel when averaged over these wave functions. Note that we derived the limiting forms of Eq. (10) by forcing only  $\epsilon_{xc}$  and the electrostatic energy to cancel. We should point out that the low-density form of  $g(n)$  proposed by Perdew and Datta<sup>15</sup> is not consistent with their  $\epsilon_{xc}$  according to this criterion.

#### IV. RESULTS IN TWO DIMENSIONS

(i) *Dielectric-function method.* In the previous section we showed that the dielectric-function method and the more general treatment allowing for finite distortions yield very similar results for three-dimensional jellium. For the two-dimensional systems discussed in this section only the simpler dielectric-function calculations have been made: These should at least give a lower limit to the transition density.

For an ideal two-dimensional gas an equation analogous to Eq. (11) can easily be written

$$F(x) = 2.51 n^{1/2} / (1.00 - 1/x), \quad (16)$$

$$F(x) = \begin{cases} 1 & x \leq 1 \\ 1 - (1 - 1/x^2)^{1/2} & x > 1 \end{cases}. \quad (17)$$

The solution proceeds as before, and we find an instability at  $n = 1.7 \times 10^{-3}$  a.u., or  $r_s = 17$ . (In two dimensions  $r_s$  is defined by  $\pi r_s^2 = 1/n$ .) Ceperley<sup>13</sup> finds  $r_s = 33$  for his two-dimensional transition, and, again a magnetic transition near  $r_s = 17$ .

Electrons in surface states on liquid helium are a very good approximation to an ideal two-dimensional electron gas, and recent experiments indicate that at

low enough temperatures Wigner crystallization occurs.<sup>17</sup> The transition observed is not the one we have been discussing which corresponds to the melting of the crystal due to zero-point kinetic energy. Rather, what has been observed is the melting due to thermal effects at very low densities. The sketch of a phase diagram in Fig. 2 should make the relationship clear.

If we apply our theory we predict that crystallized surface electrons on helium should melt if the density is raised to about  $4 \times 10^{13} \text{ cm}^{-2}$ . Experiments in this system unfortunately can only be carried out at densities below about  $10^8\text{--}10^9 \text{ cm}^{-2}$ ; it is probably out of the question to observe the higher-density melting transition for helium surface electrons.

Another system of great interest in this connection is electrons in inversion layers in silicon. Our theory must be modified in two ways to apply here: First a trivial modification is necessary because inversion-layer electrons within a crystal should be treated in the effective-mass approximations with a statically screened Coulomb interaction. This is quickly accounted for by rescaling units: now [for Si(100) surfaces] we take  $m_t = e^2/\kappa = \hbar = 1$ , where  $m_t$  is the transverse mass in the conduction band and  $\kappa = \frac{1}{2}(\epsilon_{\text{Si}} + \epsilon_0) = 7.8$  is the average static dielectric constant of Si and SiO<sub>2</sub>.

A less trivial change must be made to account for the multivalley band structure of Si. It is reasonable to suppose that the kinetic-energy term in Eq. (2) will be strongly affected by the valley degeneracy; in fact  $T$  will be reduced by the factor  $V^{-3/2}$  where  $V$  is the number of valleys. However,  $\epsilon_{\text{sc}}$  should hardly be affected at all because, as above, we are dealing

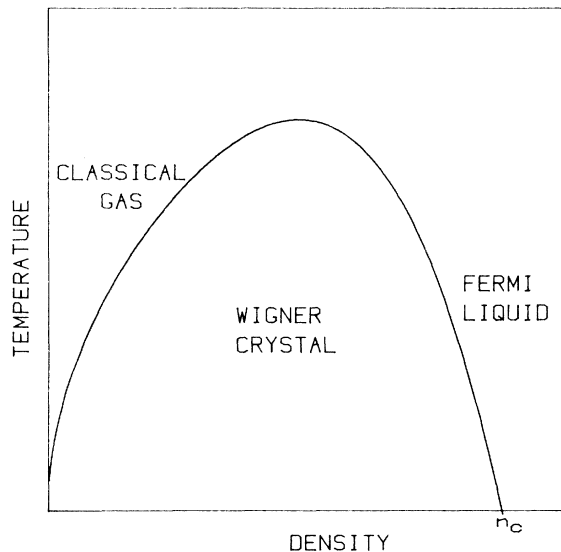


FIG. 2. Hypothetical phase diagram for electron crystallization.

mainly with corrections which should not depend strongly on valley labels. In analogous cases in studies of the electron-hole liquid<sup>18</sup> it has been found that even at high density the sum of exchange and correlation energies does not depend much on the distribution among valleys. Our approximation is to leave  $\epsilon_{\text{sc}}$  unaltered in the multivalley case.

The dielectric function calculation can now be redone for Si(100) inversion layers. We find a transition at  $n_c = 9.8 \times 10^{-4} = 2.1 \times 10^{10} \text{ cm}^{-2}$ ; i.e.,  $r_s = 18$ . The reason why the multivalley structure hardly shifts the transition in reduced units is that there is a competition of two effects: The reduction in kinetic energy due to the many-valley structure and the reduction in Fermi wave vector which means that at fixed  $q$  the argument,  $x$ , of  $\chi_0$  will be larger. For  $V = 6$ , we find  $r_s \approx 18$ , again.

This transition may be difficult to observe for the opposite reason from the one above: The range of experimental densities is usually higher than  $n_c$ . At low density it is believed that single-particle effects such as localization due to the random field of impurities near the interface dominate the electronic properties.<sup>19</sup> Conceivably the problem could be overcome by careful sample preparation.

We should note another difficulty in making an observation on this system: We require  $T < T_F$  for the electrons to remain degenerate. At  $n_c$  we find  $T_F \approx 1.5 \text{ K}$ .

Another candidate two-dimensional system is the electron gas in semiconductor heterostructures such as GaAs-GaAlAs. For this case the situation is simpler than in Si because GaAs is a direct-gap, single-valley material. We use<sup>20</sup>  $m^* = 0.067m_e$  and  $\kappa = 12.9$  to arrive at the conclusion that instability should occur for  $n_c \approx 1 \times 10^9 \text{ cm}^{-2}$ . Note that we use the low-frequency dielectric constant: The effects of ionic polarization are fully taken into account in this way. At this density  $T_F \approx 0.4 \text{ K}$ . To our knowledge experiments at this low temperature and electron density have not been performed.

(ii) *Valley density waves.* For the case of Si inversion layers several authors<sup>21,22</sup> have suggested another instability analogous to a spin-density wave, namely, a state where the valley occupancy varies in such a way as to leave the total density constant. In the low-density regime, however, such theories are open to the same objection as spin-density waves: In a regime where exchange is less important than correlation the interaction will not depend much on valley labels. In that situation as in the magnetic case, the leading instability will probably be the analog of ferromagnetism, i.e., the uniform piling up of electrons in a valley, and even that will tend to be suppressed by correlations.

The detailed calculations of Rice and Beni<sup>23</sup> on Si(111) inversion layers tend to support this qualitative argument even in a rather high-density regime.

Kalia and Quinn<sup>22</sup> explicitly demonstrate that the difference between intravalley and intervalley exchange potentials drives the transition: We believe both terms in this quantity to be quite small. If correlation is included the difference remains small though each term may be sizable.

A final comment should be made on the change in our results which might occur due to the finite thickness of the electron layers in the quasi-two-dimensional systems we have discussed. As Jonson<sup>24</sup> and others have pointed out, for small interelectron spacing the ground-state motion normal to the layer leads to an interaction far from  $1/r$ , and changes in many collective properties. However, this effect is negligible at low densities since the electrons would very seldom be in one another's vicinity. In fact, we would expect corrections to our theory to be proportional to  $\eta = \pi t^{1/2}$  where  $t$  is the layer thickness. For example, for a heterostructure with  $t \approx 100 \text{ \AA}$ ,  $\eta \approx 10^{-2}$  at the CDW transition. The situation is similar for Si inversion layers: In this system the interparticle potential approaches<sup>24</sup>  $e^2/\kappa r$  if  $r \gg t$ , as we assumed above. For electrons on liquid helium  $n_c$  is so large that our approximations would be invalid there, but in any case, there seems to be no hope of attaining such densities in practice.

## V. SUMMARY

We have applied the density-functional theory to a variety of situations to attempt to find a case where the ideas of Wigner on electronic instability against crystallization might be seen to apply. For the three-dimensional case we have no particular hope that this sort of charge-density wave will ever be observed. The results of Sec. III are mainly of interest as an example of the differing results that can be derived from different approaches to the many-electron problem.

Two-dimensional electron gases are quite a different case: Many of the cases we investigated are tantalizingly close to the practical regime of density and temperature. We believe that low-density, low temperature experiments on inversion layers and heterostructures are well worth pursuing.

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