Ground state of electron-hole droplets*

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The free-particle state corresponding to the ground state of a plasma in a band structure composed of (a) v valleys, (b) two valleys of different masses, (c) one "anisotropic" valley is studied. The Hartree-Fock approximation leads, for (a) and (b), to only one filled valley. Only *intervalley correlations* restore the unperturbed ground state (a), or a state close to (b), and make the droplets stable. For (c), the state is slightly more spherical than the free-particle ground state, but, in the three cases, the energy is not significantly changed.

I. INTRODUCTION

The usual way[1,2] of calculating the ground-state energy of a system of particles with a Coulomb interaction (V_{Coul}) is to take the ground state $|0\rangle$ of the Hamiltonian H_0 of the free-particle system, to introduce the perturbation V_{Coul} adiabatically, and to calculate the energy of the perturbed state $|\tilde{0}\rangle$ corresponding to the total Hamiltonian $H = H_0 + V_{\text{Coul}}$. When V_{Coul} changes the unperturbed energy only slightly, we may think that $|0\rangle$ leads to the real ground state of H, but when the Coulomb energy (the sum of the exchange and correlation energy) is larger, it is not obvious that another state $|0'\rangle$, an excited state of H_0, will not lead to a lower energy than $\langle\tilde{0}|H|\tilde{0}\rangle$. It is this point that we want to study in this paper for three different band structures: (a) v valleys of the same mass, (b) two valleys of different masses, and (c) one "anisotropic" valley. We will show that the *intervalley* correlations play a crucial role in determining the ground state and stabilizing the droplets.

In the first case, $|0\rangle$ leads in fact to the real ground state but this is only due to the *intervalley* correlation terms. In the two other cases, $|0'\rangle$ is a state close to $|0\rangle$ but still different: The Coulomb energy varies slowly with $|0'\rangle$ compared to the kinetic energy, so that the free-particle model is not so bad for finding the ground state (even if the energy is completely wrong).

Different methods have been used by various authors[3-6] for the calculation of the electron-hole plasma energy. In this paper, all the correlation energies E_{corr} are calculated by the Nozières and Pines[1,3] method: E_{corr} is written $E_{\text{corr}}(r_s) = \int I(q, r_s)\,dq$.

For small q, $I(q, r_s)$ takes into account all the random-phase-approximation (RPA) terms which can be summed as

$$I(q, r_s) = \frac{-q^2}{4\pi^2}\int \frac{d\omega}{2i\pi}\left[\frac{4\pi e^2}{q^2}S(q,\omega) + \ln\left(1 - \frac{4\pi e^2}{q^2}S(q,\omega)\right)\right], \quad (1)$$

where $S(q, \omega)$ is the usual correlation function

$$S(q,\omega) = \sum_k \frac{2(\epsilon_k - \epsilon_{k+q})n_k(1-n_{k+q})}{(\epsilon_{k+q}-\epsilon_k)^2 - (\omega - i\delta\,\mathrm{sgn}\omega)^2}. \quad (2)$$

For large q, $I(q, r_s)$ contains only the second-order terms (direct and exchange). For the intermediate region ($q \simeq k_F$), all the terms are important, but as it is not possible to sum all of them, the assumption is to interpolate between the small and large q values of $I(q)$. We may estimate at 10% the error on E_{corr} due to this interpolation,[7] but the relative variations of E_{corr} with respect to parameters ($r_s, \ldots$) are known with a much better precision (a few percent of the correlation energy).

II. v VALLEYS WITH THE SAME MASS m

Let us first look at a system of N electrons (and no holes) and neglect any coupling between valleys (which corresponds to the Hartree-Fock approximation or to any summation of diagrams which do not include inter-valley correlations). If the total energy of N_1 electrons in one valley is given by

$$E_1 = N_1 F(me^2/N_1^{1/3})me^4/2\hbar^2\epsilon^2,$$

where ϵ is the static dielectric constant, the total energy of N electrons in v noninteracting valleys is just the sum of the energy of each valley $E_v = NF(v^{1/3}me^2/N^{1/3})$ Ry. Thus E_v/N has the same minimum as E_1/N_1: For a density small enough ($r_s > r_0$ on Fig. 1) it is clear that the ground state corresponds to only one filled valley (or a linear combination of such states in order to restore the symmetry).

This surprising conclusion disappears if the intervalley correlations are taken into account. For a given number of electrons, $|E_v|/N$ always increases with the number of valleys (Fig. 1). A way of understanding why these correlation terms are very important is to realize that their main contribution comes from electrons near the Fermi surface. One electron near the Fermi surface may interact with $vk_F^2 \propto v^{1/3}N$ other electrons near the Fermi surface, which increases with the number

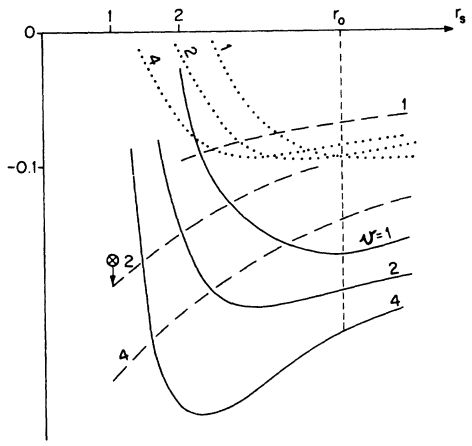

FIG. 1. E_{HF} (dotted line), E_{corr} (dashed line), and $E_{HF}+E_{corr}$ (solid line) in Ry as a function of r_s for N electrons in v valleys. ⊗ corresponds to the value obtained by changing e^2 in ve^2 in E_{corr} ($v=1$). Since the exchange diagrams are over counter, E_{corr} is underestimated by 10%.

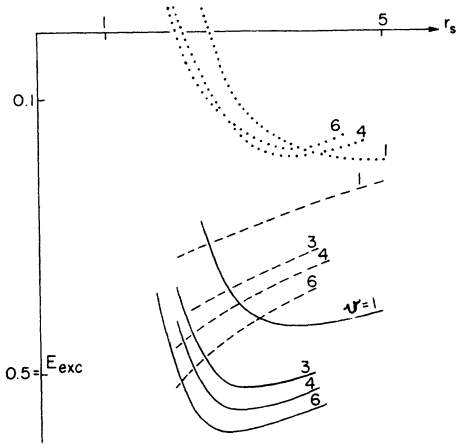

FIG. 2. E_{HF} (dotted line), E_{corr} (dashed line), and $E_{HF}+E_{corr}$ (solid line), in Ry for a plasma with v electronic valleys and one valence band of the same mass.

of valleys as $v^{1/3}$. (In fact the correlation energy increases a little faster than $v^{1/3}$, while this simple argument corresponds to considering only the static correlation function which gives the leading term for small momentum excitation.)

In conclusion, the ground state has all valleys filled as predicted by the consideration of E_{kin} alone: even if the Coulomb energy is dominant it is very slowly varying with v compared to E_{kin} [Fig. 3(a)].

Turning to a plasma with N electrons of mass m in v valleys and N holes of the same mass in one band, the Hartree-Fock energy given by

$$\frac{E_{HF}}{N}=\left[\frac{2.21(1+1/v^{2/3})}{r_s^2}-\frac{0.916}{r_s}\left(1+\frac{1}{v^{1/3}}\right)\right]\text{Ry} \quad (3)$$

has a minimum for $v=1$, so that the ground state would correspond to only one filled valley. Here too, our calculation shows that the intervalley correlations restore the expected ground state: the bigger v is, the more bound is the plasma (Fig. 2). Note that for $v\geq 3$, the binding energy of the plasma is greater than the binding energy of the exciton so that droplets become stable, and also the relative increase of the correlation energy with v is smoothed by the presence of the holes.

Our simple argument leads to a variation of the correlation energy as $1+v^{1/3}$, instead of $v^{1/3}$, which agrees surprisingly well with the numerical results.

Turning now to germanium, where we know that droplets exist, the correlation energy is $1.2\,E_{exciton}$. Univalley unimass structure gives $0.5\,E_{exciton}$. Including only valley effects ($v_e=4$, $v_h=2$) gives 0.9, other band-structure features (various masses, anisotropy, and hole coupling) giving the rest. Thus intervalley correlations appear to be the most important physical mechanism giving rise to droplets.

III. TWO VALLEYS WITH DIFFERENT MASSES (m_H and m_L)

This situation may appear, for instance, in the droplets of GeSi (Ref. 8) (for 15% of Si the two types of conduction band have the same minimum). Looking at the binding energy of the exciton, one might think that droplets made only with the heavier band would be more stable than those corresponding to a situation in which both valleys are filled up to the same Fermi level. In order to see a pure effect (not smoothed by the holes) we will only consider N electrons and no holes. The unperturbed ground

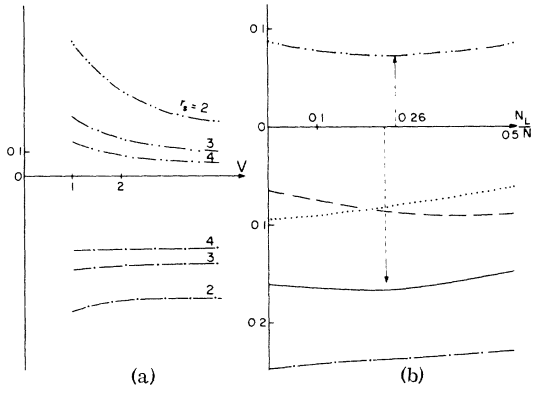

FIG. 3. (a) E_{kin} (double-dot–dashed line), $E_{exch}+E_{corr}$ (dot-dashed line), as a function of the number of valleys. (b) E_{kin} (double-dot–dashed line), E_{HF} (dotted line), E_{corr} (dashed line), $E_{HF}+E_{corr}$ (solid line) and $E_{exch}+E_{corr}$ (dot-dashed line) of N electrons in two bands as a function of the initial number of electrons N_L in the lightest band ($r_s=5$, $m_H=2m_L$ is the unit of mass).

state will be taken with the heaviest (lightest) band filled up to a Fermi momentum k_H (k_L).

Taking m_H and $k_0 = (3\pi^2 N)^{1/3}$ as units, the Hartree-Fock energy can be written

$$\frac{E_{HF}}{N} = \frac{2.21(k_H^5 + k_L^5/m_L)}{r_s^2} - \frac{0.916(k_H^4 + k_L^4)}{r_s}. \quad (4)$$

Adding the equation for the conservation of electrons $k_H^3 + k_L^3 = 1$, one finds that the lowest energy corresponds to ($k_H = 1$, $k_L = 0$): All the electrons must be in the heaviest band.

There again, it may be advantageous to fill the lightest band because of intervalley correlation. Using our simple argument, E_{corr} is a maximum when the density of states near the Fermi surface $k_L^2 + k_H^2$ is a maximum so that $k_H = k_L$. In fact the calculation shows that the correlations fill up the lightest band: the ground state corresponds to $k_H^2/m_H \gtrsim k_L^2/m_L$, so the energy does not change significantly from the free-electrons ground state (even if $m_H = 2m_L$).

From Fig. 3(b) one notes that the Coulomb energy is a slowly varying quantity compared to the kinetic energy so that the latter one determines the ground state.

IV. ONE ANISOTROPIC VALLEY

We now consider electrons with an energy $\epsilon(k) = k_\parallel^2/2m_\parallel + k_\perp^2/2m_\perp$. As pointed out by Kohn and Luttinger,[9] symmetry arguments suggest that adding a Coulomb potential which has a spherical symmetry to a Hamiltonian with an ellipsoidal symmetry will give rise to a system with a symmetry more spherical than the initial ellipsoid. In order to examine this point more carefully, we will use a set of initial states $|0'\rangle$ defined by a density of state $n_k = \Theta((3\pi^2 N)^{2/3} - s^2 k_\parallel^2 - k_\perp^2/s)$ (which is not of course the most general possible $|0'\rangle$, but leads to tractable calculations and provides sufficient physical insight). s is a variational parameter taken in the range $m_\perp/m_\parallel = \rho < s^3 < 1$. Using $k_0 = (3\pi^2 N)^{1/3}$ and $m_\perp$ as units, the Hartree-Fork energy is

$$\frac{E_{HF}}{N} = \frac{2.21}{r_s^2}\frac{s}{3}\left(\frac{\rho}{s^3} + 2\right) - \frac{0.916}{r_s}\left(\frac{s}{1-s^3}\right)^{1/2} \times \arcsin(1-s^3)^{1/2}. \quad (5)$$

As shown in Fig. 4, E_{HF}/N has a minimum for s^3 bigger than ρ (if $\rho = 0.05$, $s^3 \simeq 0.13$).

The calculation of the correlation energy is very tedious but may be performed analytically, except for the form factor. One finally finds that, here again, correlations cancel a part of the modification of the ground state due to exchange: the real ground state remains, as expected, a little more spherical than the free-particles one ($s^3 \simeq 0.09$ for $\rho = 0.05$) but the change in energy is insignificant, even in the case of large anisotropy (Fig. 4). As correlations correspond to screen the Coulomb potential, it is reasonable to find that they tend to leave the original anisotropy unchanged. The inclusion of holes tends to smooth all the effects so that this conclusion will clearly remain true for the calculation of the energy of electron-hole droplets.

One can conclude that the free-electrons ground state leads to a correct value of the binding energy of the plasma (the modification being within the uncertainties due to the usual calculation of the correlation energy). The reason for this is that the intervalley correlation terms cancel the variation of the exchange energy and lead to a Coulomb energy which is very slowly varying with $|0'\rangle$ compared to the kinetic energy: as we know the free electron model is not such a bad one!

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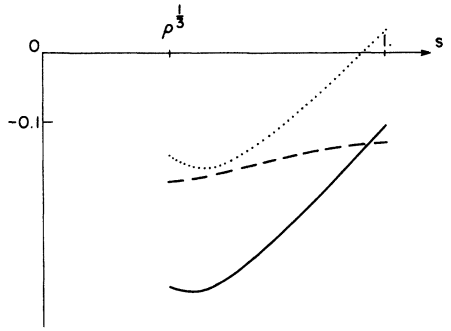

FIG. 4. E_{HF} (dotted line), E_{corr} (dashed line), and $E_{HF} + E_{corr}$ (solid line) for an anisotropic electron gas (with $\rho = \frac{1}{20}$) as a function of the anisotropy s of the initial state.

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compatible with the slope of $E_c(r_s)$. This way, we obtain for the binding energy of the droplets for Ge, 5.7 meV and for Si, 19.4 meV.

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