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LETTER TO THE EDITOR

Dimensional instabilities of an electron gas in a quantum dot

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Abstract. Instabilities are found in an interacting electron gas confined in a three-dimensional quantum dot as a function of magnetic field. These instabilities involve transitions between one-, two- and three-dimensional electron systems. In contrast to what is found for the non-interacting electron case, these dimensional instabilities can occur in essentially isotropic quantum dots.

There has been much interest in possible instabilities in two- and three-dimensional interacting electron gases in strong magnetic fields [1] and, more recently, in two-dimensional electron gases as the third degree of freedom is introduced [2, 3]. The current level of flexibility in semiconductor microstructure design now allows the possibility of confining a three-dimensional electron gas (3DEG) in all three directions, forming so-called quantum dots [4, 5]. The strength of the confinement in the three directions is essentially a controllable parameter as is the number of electrons in the dot. The presence of image charges in nearby gates and dielectric layers can, according to the specific dot design, affect the form of the effective interaction between two electrons within the dot. The effects of the electron–electron interaction in a *two*-dimensional quantum dot lying in the xy-plane have already been shown to be significant [6–10]. Because of the computational complexity, however, little theoretical work [11] has yet been performed on the effects of the electron–electron interaction in the more realistic case of three-dimensional dots.

In this work we consider a simple, analytically solvable model of an interacting electron gas in a three-dimensional parabolic quantum dot. The model predicts that the freedom of motion of the electrons in the third (z) direction can lead to instabilities in the quantum dot electron gas. This behaviour results from the interplay of the electron–electron interaction, the Pauli exclusion principle, the single-particle confinement energy and the cyclotron energy. We show that for reasonably isotropic quantum dots, in contrast to the non-interacting electron system (i) a stable one-dimensional gas (1DEG) phase can exist for a range of magnetic fields, (ii) a two-dimensional gas (2DEG) phase can exist that is stable for *all* magnetic fields, (iii) these phases can survive in the presence of vanishingly small anisotropies either in the dot shape, or in the electron–electron interaction. Finally we discuss physically

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observable consequences of these dimensional instablities, and the validity of the present simple model.

Our model Hamiltonian for a three-dimensional quantum dot with a magnetic field $\boldsymbol{B}$ along the z-direction is a generalization of that introduced in [9]. The present Hamiltonian H allows for a wide range of possible dot parameters resulting from differing experimental designs, while still permitting analytic solutions. The dot size (i.e. parabolic curvature) in the z-direction (ω_{0z}) is allowed to differ from that in the xy-plane (ω_0). Also we attempt to mimic the effects of image charges in adjacent semiconductor layers and gates by allowing the strength of the electron–electron interaction in the z-direction (Ω_z) to differ from that in the xy plane (Ω). The electron–electron interaction potential is now given by

$$V(\boldsymbol{r}_i, \boldsymbol{r}_j) = 3V_0 - \tfrac{1}{2}m^*\Omega^2|\boldsymbol{r}_{i,\parallel} - \boldsymbol{r}_{j,\parallel}|^2 - \tfrac{1}{2}m^*\Omega_z^2|z_i - z_j|^2. \tag{1}$$

The positive parameters V_0, Ω and Ω_z can be chosen to model dots of different sizes and materials as discussed in [9]. The electron position $\boldsymbol{r}_i = (x_i, y_i, z_i) = (\boldsymbol{r}_{i,\parallel}; z_i)$. The dot contains N interacting electrons with effective mass m^*, negative charge $-e$, g-factor g^* and spin components $\{s_{i,z}\}$ along the z-axis. The momentum and vector potential associated with the ith electron are given by $\boldsymbol{p}_i$ and $\boldsymbol{A}_i$ respectively, and μ_B is the Bohr magneton. The Hamiltonian is given by

$$H = \frac{1}{2m^*}\sum_i \left(\boldsymbol{p}_i + \frac{e\boldsymbol{A}_i}{c}\right)^2 + \frac{1}{2}m^*\sum_i(\omega_0^2|\boldsymbol{r}_{i,\parallel}|^2 + \omega_{0z}^2 z_i^2) + \sum_{i<j} V(\boldsymbol{r}_i, \boldsymbol{r}_j) - g^*\mu_B B\sum_i s_{i,z} \tag{2}$$

and is separable into an xy-dependent part $H_\parallel(\{\boldsymbol{r}_{i,\parallel}\})$ and a z-dependent part $H_z(\{z_i\})$. As shown in [9], $H_\parallel$ can be diagonalized exactly by introducing centre-of-mass ladder operators ($A^\pm$ and $B^\pm$) and relative mode ladder operators ($a_{ij}^\pm$ and $b_{ij}^\pm$). Likewise H_z can be diagonalized using centre-of-mass ladder operators $C^\pm$ and relative mode ladder operators $c_{ij}^\pm$ where

$$c_{ij}^\pm = (1/2m^*\hbar\Omega_{0z})^{1/2}(m^*\Omega_{0z}z_{ij} \mp \mathrm{i}p_{ij,z}). \tag{3}$$

In this work we define $\Omega_{0z} = \sqrt{\omega_{0z}^2 - N\Omega_z^2}$, $\omega_0^2(B) = \omega_0^2 + \omega_c^2/4$, $\Omega_0(B) = \sqrt{\omega_0^2(B) - N\Omega^2}$, $\omega_c = eB/m^*c$ and m_0 is the free-electron mass. We have made the coordinate transforms $\boldsymbol{R} = (X, Y, Z) = (1/N)\sum_i \boldsymbol{r}_i$ and $\boldsymbol{r}_{ij} = (x_{ij}, y_{ij}, z_{ij}) = \boldsymbol{r}_i - \boldsymbol{r}_j$ and have defined the corresponding momentum operators $\boldsymbol{P} = (P_X, P_Y, P_Z) = \sum_i \boldsymbol{p}_i$ and $\boldsymbol{p}_{ij} = (p_{ij,x}, p_{ij,y}, p_{ij,z}) = \boldsymbol{p}_i - \boldsymbol{p}_j$. In addition, we take $\omega_{0z} > N^{1/2}\Omega_z$ and $\omega_0 > N^{1/2}\Omega$ so that all N electrons remain confined to the dot (see later). For simplicity, we consider the magnetic field, or the g-factor, to be sufficiently large that the electrons in the dot are spin polarized. In the InSb quantum dots of [4] where $\hbar\omega_0 = 7.5$ meV, for example, a field as small as 3 T is sufficient to ensure spin polarization for $N = 4$ electrons [12].

The Hamiltonian H can be solved exactly analytically. For a particular magnetic field ω_c, the ground state is a sensitive function of the strength of the electron–electron interaction, the confinement energies and the particle number. As the dot parameters are varied, there are three possible regimes (1DEG, 2DEG and 3DEG) each of which corresponds to a different dimensional behaviour of the ground and lowest excited states. We first describe these regimes, and then give the stability criterion for each.

1DEG *regime.* In this regime the motion of the electrons is confined to the z-direction and the total angular momentum J is zero. (In a non-interacting picture, the electrons would all be occupying the lowest xy-plane subband.) The electrons have reduced their mutual interaction energy by separating in the z-direction. Using the notation of [9] the ground state of H in the 1DEG regime is given by $\Psi_{1D} \equiv \prod_{i<j} c_{ij}^{+}|0\rangle$ and has a corresponding energy

$$E_{1D} = \hbar[\omega_0(B)+\tfrac{1}{2}(N-1)(N+1)\Omega_{0z}+(N-1)\hbar\Omega_0(B)+\tfrac{1}{2}\hbar\omega_{0z}-(g^*m^*/4m_0)N\omega_c] + 3N(N-1)V_0/2. \tag{4}$$

The spatial part of the corresponding wavefunction is given by

$$\Psi_{1D} = \left\{ \prod_{i<j} (m^*\Omega_{0z} z_{ij} - \mathrm{i} p_{ij,z}) \right\} \Psi_0 \tag{5}$$

where Ψ_0 is the zero-point wavefunction

$$\Psi_0 = \exp\left(-\frac{Nm^*}{2\hbar}[\omega_0(B)(X^2+Y^2)+\omega_{0z}Z^2] - \frac{m^*}{2N\hbar}\sum_{i<j}[\Omega_0(B)(x_{ij}^2+y_{ij}^2)+\Omega_{0z}z_{ij}^2] \right). \tag{6}$$

3DEG *regime.* As the magnetic field is increased, it becomes energetically favourable for the electrons to separate in the xy-plane, and the angular momentum becomes non-zero. The crossover from the 1D to 3D regimes occurs when antisymmetric combinations of states like $a_{Nk}^{+}\prod_{i<j} c_{ij}^{+}|0\rangle$ (with $i,j,k \leqslant N-1$) become lower in energy than $\prod_{i<j} c_{ij}^{+}|0\rangle$ (with $i,j \leqslant N$). The electrons are now moving in all three directions. As the magnetic field is increased further, the ground state contains increasing powers of the a_{ij}^{+} operators thereby increasing the angular momentum in the xy-plane.

2DEG *regime.* For large magnetic field, the electrons all move in the xy-plane and do not need to separate in the z-direction. (In the non-interacting picture, the electrons now essentially occupy the lowest z-direction subband. This is the limit implicitly assumed in [6]–[10].) The ground state in the 2DEG regime has a high angular momentum J, and is given by $\Psi_{2D} \equiv \prod_{i<j} a_{ij}^{+}|0\rangle$ with a corresponding energy

$$E_{2D} = \hbar[\omega_0(B)+\tfrac{1}{2}(N-1)(N+2)\Omega_0(B)-\tfrac{1}{4}N(N-1+g^*m^*/m_0)\omega_c] + 3N(N-1)V_0/2+\tfrac{1}{2}\hbar\omega_{0z}+\tfrac{1}{2}(N-1)\hbar\Omega_{0z}. \tag{7}$$

The spatial part of the corresponding wavefunction has the Vandermonde form

$$\Psi_{2D} = \left\{ \prod_{i<j} (x_{ij} - iy_{ij}) \right\} \Psi_0. \tag{8}$$

We would like to point out that this work considers sufficiently strong xy-confinement (i.e. $\omega_0 > N^{1/2}\Omega$) that the angular momentum of the ground state in the 2DEG regime corresponds to an effective filling factor [7] $\nu = 1$, i.e. $J = N(N-1)/2$, and the higher J-states are excited modes [13]. The softening of these higher J-modes when $\omega_0 = N^{1/2}\Omega$ is discussed in relation to figures 2 and 3, and is the subject of [7] and [8]. We emphasize that these higher J-states are still two-dimensional in the xy-plane [7, 8].

The stability conditions for the above 1D, 2D and 3D regimes can be expressed in terms of critical magnetic fields. We define parameters $\lambda = (\Omega_z/\Omega)^2$ and $\delta = (\omega_0/\omega_{0z})^2$ which describe the degree of anisotropy in the electron–electron interaction and the dot confinement respectively. The 1DEG regime will be stable compared to the 3DEG regime when $\omega_c < \omega_{c1}$, where

$$\omega_{c1} = \frac{\delta(\omega_0^2 - N\Omega^2) - (N-1)^2(\omega_0^2 - N\lambda\delta\Omega^2)}{(N-1)(\delta(\omega_0^2 - N\lambda\delta\Omega^2))^{1/2}}. \tag{9}$$

For $\omega_{c1} < \omega_c < \omega_{c2}$ the 3DEG is stable, where

$$\omega_{c2} = \frac{\delta(N-1)^2(\omega_0^2 - N\Omega^2) - (\omega_0^2 - N\lambda\delta\Omega^2)}{(N-1)(\delta(\omega_0^2 - N\lambda\delta\Omega^2))^{1/2}}. \tag{10}$$

For $\omega_c > \omega_{c2}$ the 2DEG is stable. For $N > 2$ electrons ω_{c1} is *always* less than ω_{c2}. In the special case $N = 2$, $\omega_{c1} = \omega_{c2}$ and no 3DEG regime exists.

Depending on the values of the parameters N, λ, δ, ω_0 and Ω, these critical fields ω_{c1} and ω_{c2} may be positive or negative. For a stable 1DEG phase to exist at finite magnetic fields, we need $\omega_{c1} > 0$ which implies

$$(\Omega/\omega_0)^2 > [(N-1)^2 - \delta]/[N\delta((N-1)^2\lambda - 1)]. \tag{11}$$

Similarly, for a 3DEG→2DEG transition to occur at finite fields, we need $\omega_{c2} > 0$ which implies

$$(\Omega/\omega_0)^2 < [\delta(N-1)^2 - 1]/[N\delta((N-1)^2 - \lambda)]. \tag{12}$$

Figure 1 shows the three possible types of behaviour (I, II and III) of an electron gas in a quantum dot as a function of magnetic field for a given choice of N, λ, δ, ω_0 and Ω. Figures 2 and 3 show the occurrence of these regions I, II and III as a function of $(\Omega/\omega_0)^2$ and the anisotropy parameters λ and δ. In figure 2 the quantum dot confinement is isotropic ($\delta = 1$) but the electron–electron interaction is allowed to be anisotropic. In figure 3 the electron–electron interaction is isotropic ($\lambda = 1$) but the confinement can be anisotropic. The boundaries between regions I, II and III in figures 2 and 3 can easily be obtained from (11) and (12) by setting $\delta = 1$ and $\lambda = 1$ respectively. The most surprising conclusions from figures 2 and

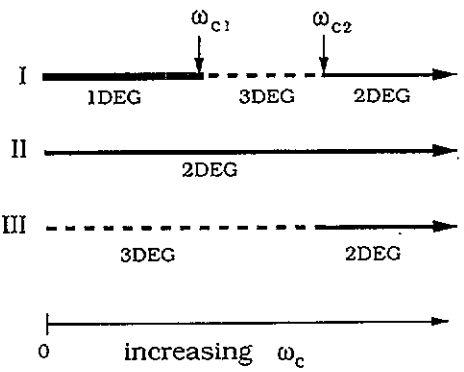

Figure 1. The three possible types of behaviour (I, II and III) of an interacting electron gas in a quantum dot as a function of magnetic field ω_c.

3 are that, for vanishingly small anisotropies (i.e. $\lambda, \delta \to 1$) in the quantum dot, (i) a 1DEG phase exists for $\omega_c < \omega_{c1}$ (region I), and (ii) the interacting electron gas can have a stable 2DEG phase for all magnetic fields (region II). We emphasize that for a *non-interacting* electron gas (i.e. $\Omega = 0$), the behaviour in figure 2 is always described by region III and is independent of λ. From figure 3, the non-interacting electron gas in a reasonably isotropic dot (i.e. $\delta \sim 1$) also corresponds to region III. A non-interacting electron gas will only yield a 1DEG phase for extremely anisotropic dots, i.e. when $\delta > (N-1)^2$ which for $N = 4$ implies $\delta > 9$. Likewise, a 2DEG phase that is stable for all magnetic fields will form only if $\delta < (N-1)^{-2}$, which for $N = 4$ implies $\delta < 0.11$. An extreme numerical example of the difference between the interacting and the non-interacting electron gas in a dot is as follows. Consider the InSb dot with $N = 4$, $\hbar\omega_0 = 7.50$ meV, $\hbar\omega_{0z} = 4.33$ meV (i.e. $\delta = 3$), $\hbar\Omega = 1.53$ meV and $\hbar\Omega_z = 2.16$ meV (i.e. $\lambda = 2$). The 1DEG phase is stable up to 12.5 T. In the non-interacting electron gas the 1DEG is *always* unstable. Likewise, the interacting electron gas would only form a 2DEG phase above 112 T while the non-interacting system would form a 2DEG phase above 4.5 T!

Regions IA and IIA in figures 2 and 3 correspond to the regimes $\omega_{0z} < N^{1/2}\Omega_z$ and $\omega_0 < N^{1/2}\Omega$ respectively where higher-energy modes become soft. The thick boundary line between I and IA is given by $(\Omega/\omega_0)^2 = (N\lambda\delta)^{-1}$, while that between II and IIA is given by $(\Omega/\omega_0)^2 = N^{-1}$. In regions IA and IIA, the N-electron gas within our model is energetically unstable to loss of one electron, forming an $N-1$ electron gas. For an electron–electron interaction of more *Coulombic* form, the Nth electron would not actually leave the dot. Instead it would settle in an orbit of large radius, hence forming a new ground state of the same dimensionality. Region IIA in figure 2 would correspond to a 2DEG phase with large angular momentum (i.e. $\nu < 1$) as discussed in [7] and [8]. Similarly region IA would correspond to a new 1DEG phase along the z-direction.

We will illustrate the physical consequences of the above dimensional instabilities by commenting on the difference between the 1DEG and 2DEG regimes. There are low-lying energy excitations in the 2DEG regime with angular momenta $\Delta J = 1, 2, \ldots$, above the ground-state value $N(N-1)/2$. These excitations have energies of the form

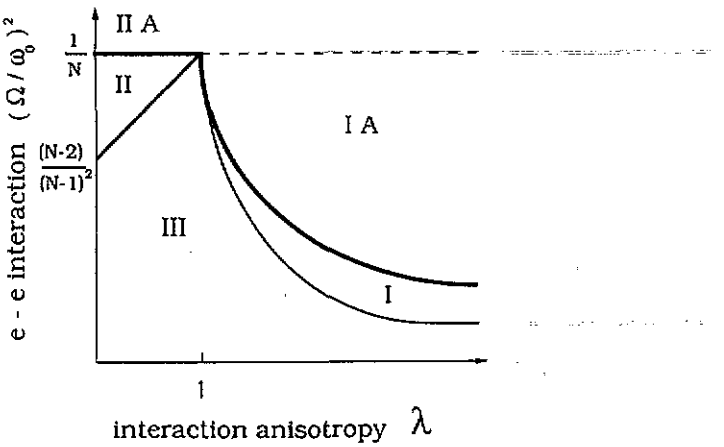

Figure 2. Regions I, II and III as a function of the scaled electron–electron interaction $(\Omega/\omega_0)^2$ and the electron–electron interaction anisotropy λ. The dot confinement is isotropic ($\delta = 1$).

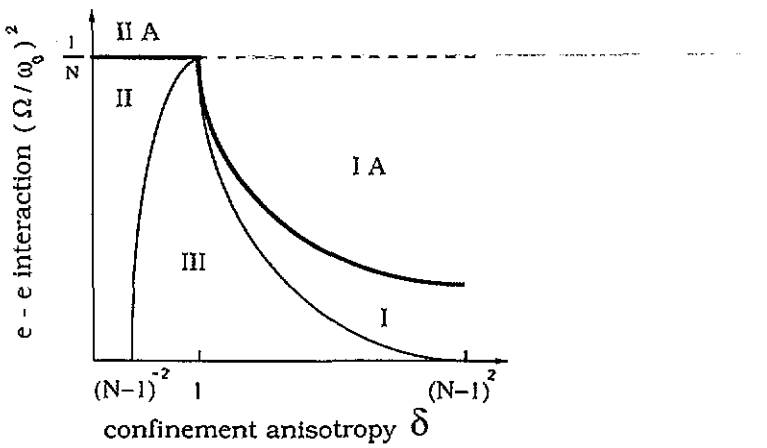

Figure 3. Regions I, II and III as a function of $(\Omega/\omega_0)^2$ and the dot confinement anisotropy δ. The electron–electron interaction is isotropic ($\lambda = 1$). The non-interacting electron gas corresponds to the $(\Omega/\omega_0)^2 = 0$ axis.

$$\Delta E_{2D} = n\hbar(\omega_0(B) - \omega_c/2) + m\hbar(\Omega_0(B) - \omega_c/2) \tag{13}$$

where n and m are non-negative integers such that $n + m = \Delta J$. The excitation energies in (13) can depend strongly on the magnetic field strength. We note that the antisymmetry requirement on the total N-electron wavefunction leads to missing modes, e.g. $m = 1$ (see in [13]). By contrast the low-lying excitations in the IDEG regime correspond to $J = 0$. The corresponding energies are independent of the magnetic field strength, and are of the form

$$\Delta E_{1D} = n\hbar\omega_{0z} + m\hbar\Omega_{0z} \tag{14}$$

where the integers n and m no longer satisfy $n + m = \Delta J$. The magnetic field

dependence of optical transition energies and various thermodynamic properties such as heat capacity will therefore differ for the 2DEG and 1DEG regimes.

We now discuss the validity of the present model. Many recent far-infrared absorption measurements (e.g. [4]) have shown that the experimental x–y confinement is nearly parabolic, based on the generalized Kohn theorem [14, 7]. As shown in this paper, the additional use of a parabolic confinement in the z-direction, together with a harmonic electron–electron interaction, enables analytic solutions to be obtained for the otherwise complicated, three-dimensional many-body problem. The actual form of the experimental z-confinement potential will depend strongly on the specific device design, as borne out by detailed numerical calculations [11]. However, if limited diffusion of the (z-direction) double barrier is allowed during the growth of the vertical-transport structures of Tewordt *et al* [5], a roughly parabolic z-confinement potential could be prepared. The resulting magnetic-field dependence of the conductance peaks (i.e. energy levels) of such structures would differ dramatically according to the value of the confinement anisotropy δ, as discussed above. The harmonic electron–electron interaction is obviously not correct for all electron separations r, but the interaction parameters can be adjusted to give the best fit to the true interaction for the dominant range of r [9]. We note that the present model yields reasonable agreement with [7] and [15] for the excitation spectra of $N \leqslant 4$ electrons in small *two*-dimensional dots, suggesting that the overall physics is not too sensitive to the form of the interaction for small dots. The present model can also describe the previously mentioned fractional ground states (i.e. $\nu < 1$) of [7] and [8] *if* the next term in the Taylor series of a cut-off Coulomb interaction $|r_i - r_j|^4$ is included in perturbation theory [16].

Despite the over-simplified form of the present model, we believe that the results obtained warrant future experimental (and numerical) investigation into dimensional instabilities in quantum dot samples.

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