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Wigner Crystalization in Semiconductor Quantum Wires

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Abstract

We study the Wigner crystallization in semiconductor quantum wires within the density functional approach. As the density of electrons in quasi-one-dimensional structures is lowered, we find that the system favors the crystalline phase as envisioned by Wigner.

The quasi-one-dimensional (Q1D) electron gas models are of great interest because of theoretical and technological implications. The motion of electrons confined to move freely only in one spatial dimension gives rise to a variety of interesting phenomena. The many-body effects in quantum wires are recently gaining importance as the fabrication techniques continue to improve. In this work we investigate the possibility of fluid to solid phase transition in a Q1D electron system at low densities. The so-called Wigner transition[1,2] occurs at zero temperature and at a critical density when the Coulomb energy becomes much larger than the kinetic energy. Our chief aim in this work is to provide with an estimate on the Q1D electron density at which a Wigner solid forms within a simple jellium model using the available exchange-correlation energies. We find that semiconductor based heterostructures out of which Q1D electronic systems can be formed promises to be a likely candidate to observe the quantum freezing transition in a one-dimensional (1D) electron system.

The density functional theory of freezing of quantum liquids has been quite successful in predicting the critical values of thermodynamic parameters at the liquid-solid transition and in describing the nature of the transition. The pioneering work of Ramakrishnan and Yussouff[3] as developed by Senatore and Pastore[4] with application to quantum systems sets the theoretical framework for the present study. The ground state energy E_0 of a many electron system can be written as a functional of the electron density $\rho(\vec{r})$ as

$$E_0 = \int d\vec{r}\{t[\rho(\vec{r})] + u[\rho(\vec{r})] + \varepsilon_x[\rho(\vec{r})] + \varepsilon_c[\rho(\vec{r})]\} + \int d\vec{r}\, V_{ext}[\rho(\vec{r})]\,, \qquad (1)$$

where t is the kinetic energy, u is the Coulomb interaction potential, ε_x and ε_c are the exchange and the correlation energies, respectively, and V_{ext} is the externally applied potential, which is taken to be zero in this work. We choose to follow the previous examples[5,6] which yield reasonable estimates for Wigner crystallization in higher dimensions. The kinetic energy functional within the Thomas-Fermi-Weizsäcker approximation in 1D can be expressed in atomic units (a. u.) as

$$t[\rho] = C_k \rho(z)^3 + \frac{1}{8} \frac{\vec{\bigtriangledown}\rho(z)\vec{\bigtriangledown}\rho(z)}{\rho(z)}\,, \tag{2}$$

where $C_k = \pi^2/24$, and the potential energy by

$$U(z) = \frac{1}{2} \int dz' \frac{[\rho(z') - \rho_0][\rho(z') - \rho_0]}{[\ b^2 + (z - z')^2\ ]^{1/2}}\,, \tag{3}$$

where ρ_0 is the homogeneous electron density, b is the model dependent quantum wire width. In this work, we use the cylindrical quantum wire model developed by Gold and Ghazali,[7] thus, the electrons are confined to have free motion in the axial direction (z-axis) of the cylinder with radius $R = b$. We also assume that only the lowest subband of the 1D electron gas is populated which becomes valid for $r_s \geq b/4a_B^*$.

For the exchange and correlation energies we employ a Padé approximation to obtain an analytical fit to the ground-state energy results obtained by Calmels and Gold[8] for a Q1D electron gas. We obtain

$$E_{\rm x}[\rho] = -\frac{1}{2} a_0 \int dz\, \rho(z)\, \frac{1 + a_1 r_s + a_2 r_s^2}{1 + a_3 r_s + a_4 r_s^2 + a_5 r_s^3}\,, \tag{4}$$

$$E_{\rm c}[\rho] = -\frac{1}{2} c_0 \int dz\, \rho(z)\, \frac{-1 + c_1 r_s + c_2 r_s^2}{1 + c_3 r_s + c_4 r_s^2 + c_5 r_s^3}\,, \tag{5}$$

in which $\{a_i\}$ and $\{c_i\}$ are parameters that depend on the wire radius, shown in Table 1. The Wigner-Seitz radius r_s for a one-dimensional system is defined as $r_s = 1/(2\rho_0 a_B^*)$, where a_B^* is the effective Bohr radius.

To describe the inhomogeneous density distribution, we consider a small modulation of the density around ρ_0 described by

$$\rho(z) = \rho_0[1 + \lambda \cos(qz)]\,, \tag{6}$$

where λ is a small parameter ($\lambda \ll 1$), and q represents a wave vector for density modulation in 1D. Such an ansatz to the inhomogeneous density provided[5] a good estimate for the Wigner transition in 2D. We assume that the electrons will be equidistant on a straight line in the solid phase which gives $q = 2\pi/r_s$. By making use of Eqs. (1)-(5), one gets the energy difference between the solid (inhomogeneous) and liquid (homogeneous)

Table 1. The exchange and correlation energy coefficients for quantum wire of radius $b = 0.5\,a_B^*$ and $b = a_B^*$.

b/a_B^*	a_0	a_1	a_2	a_3	a_4	a_5
0.5	4.80426	22.9817	9.611592	29.2405	84.5466	15.1783
1.0	2.4023	13.4298	3.5108	16.5626	26.2247	2.8945
b/a_B^*	c_0	c_1	c_2	c_3	c_4	c_5
0.5	0.0133105	15.6936	29.9494	0.499742	1.01564	0.132745
1.0	0.00314	13.6338	61.2866	0.5366	0.63904	0.07028

phases ($\Delta E = E_s - E_l$), the energy difference per particle ($\Delta\varepsilon = \Delta E/\rho_0 \int dz$) in a. u. is

$$\begin{aligned}\frac{\Delta\varepsilon}{\lambda^2} &= C_k\rho_0^2 + \frac{1}{16}q^2 + \frac{1}{2}\rho_0 K_0(qb) - \frac{1}{4}\left(\frac{a_0}{\rho_0}\right)\left[\frac{CD - BE - A(F-E)}{D^2}\right] \\ &- \frac{1}{4}\left(\frac{c_0}{\rho_0}\right)\left[\frac{IJ - HK - G(L-K)}{J^2}\right], \end{aligned} \tag{7}$$

where $K_0(x)$ is the modified Bessel function of zeroth order. The first set of coefficients $(A - G)$ are explicitly given by

$$\begin{aligned} &A = \rho_0(1 + \tfrac{1}{2}a_1\rho_0 + \tfrac{1}{4}a_2\rho_0^2), \qquad B = \tfrac{1}{2}\rho_0(1 + a_1\rho_0 + \tfrac{3}{4}a_2\rho_0^2), \\ &C = \tfrac{1}{2}\rho_0(a_1\rho_0 + \tfrac{3}{2}a_2\rho_0^2), \qquad D = 1 + \tfrac{1}{2}a_3\rho_0 + \tfrac{1}{4}a_4\rho_0^2 + \tfrac{1}{8}a_5\rho^3, \\ &E = \tfrac{1}{2}\rho_0(a_3 + a_4\rho_0 + \tfrac{3}{4}a_5\rho_0^2), \quad F = \tfrac{1}{4}\rho_0(a_4\rho_0 + \tfrac{3}{2}a_5\rho_0^2) \\ &G = \rho_0(-1 + \tfrac{1}{2}c_1\rho_0 + \tfrac{1}{4}c_2\rho_o^2). \end{aligned} \tag{8}$$

The second set of coefficients $(H - L)$ can be obtained from the first set by interchanging $\{a_i\}$ and $\{c_i\}$.

We plot $\Delta\varepsilon/\lambda^2$ in Eq. (7) as a function of the density parameter r_s in Fig. 1. The freezing point is determined to occur at $r_{sc} = 5.355$ for wire radius $0.5\,a_B^*$ and at $r_{sc} = 5.717$ for wire radius a_B^*. These values are in good agreement with the excitonic Wigner crystal calculations of Ivanov and Haug for comparable structures[9]. We were not able to obtain a transition to the ordered phase for quantum wires of radius $b \geq 2\,a_B^*$. This, however, may be partly due to the approximate nature of the correlation energy. Currently produced quantum wires have densities of $r_s \approx 1$, but it is conceivable that advances in the fabrication techniques will lead to the observation of Wigner crystallization in such structures. The exchange-correlation energies we use are based on the self-consistent field method [8] which may underestimate the exact values.

In summary, we have examined the possibility of Wigner crystallization in quantum wire systems, within a density functional theory approach, using the correlation energy

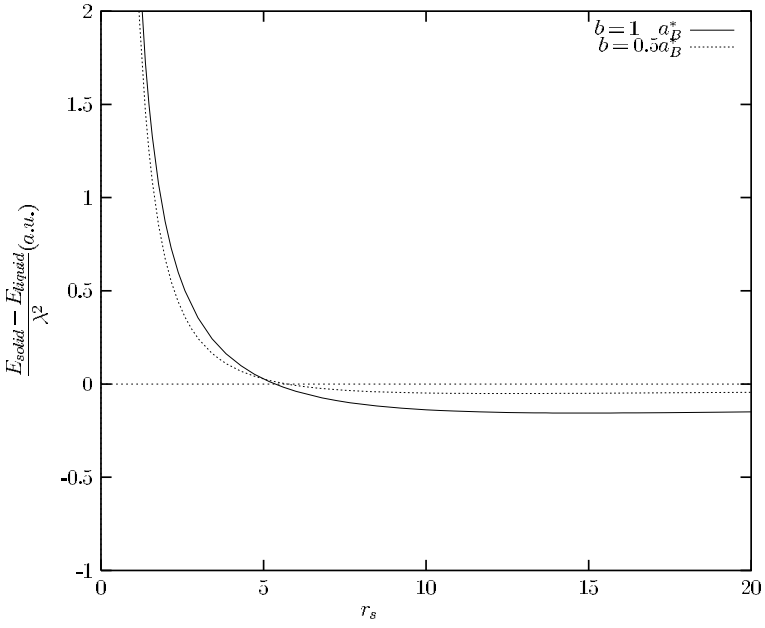

Figure 1. The difference in the average energy per particle $(\varepsilon_{\rm solid} - \varepsilon_{\rm liquid})/\lambda^2$ (in a. u.) as a function of r_s for a single quantum wire of radius $b = 0.5\, a_B^*$ (solid line) and $b = a_B^*$ (dotted line).

given by the self-consistent field scheme [8]. In view of the importance of the correct liquid state input in the density functional theories of freezing, it would be most useful to have accurate ground state energies and structure factors for Q1D electron systems in the more accurate QMC and hyper-netted chain type calculations. Since the disorder effects significantly alter the Wigner crystallization picture [10], it would be interesting to investigate similar mechanisms in Q1D structures.

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