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Quantum fluctuations in a quantum dot array in the regime of ferroelectric phase transitions

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Abstract. Quantum fluctuations in a molecular-like array of quantum dots undergoing ferroelectric (antiferroelectric) phase transitions are considered. We calculate the spectrum of collective excitations and investigate the behaviour of soft modes in the vicinity of the phase transitions. The amplitude of quantum fluctuations as a function of parameters of the system is found. We show that an external magnetic field can induce phase transitions and suppresses quantum fluctuations.

1. Introduction

Spontaneous electron polarization of two-dimensional arrays of quantum dots is discussed in the current literature [1, 2, 3, 4]. Such a phenomenon may arise from interdot Coulomb interaction and was predicted for quantum dot arrays with a parabolic confinement [1, 2] and for the arrays with a complex elementary cell [3, 4]. In particular, the authors of [3] have considered so-called quantum cellular automata based on Coulomb interaction between quantum dots. A molecular-like array of quantum dots has been proposed in [4] to show the possibility of ferroelectric (antiferroelectric) phase transitions.

In the present paper, we exploit the model of a molecular-like array of quantum dots [4] to study quantum fluctuations in the ferroelectric (antiferroelectric) state. Quantum fluctuations play an important role in the problem of phase transitions [5], because they may, in principle, destroy the ferroelectric ordering. We show in this paper that, despite fluctuations, ferroelectric (antiferroelectric) phases can exist in the molecular-like array of quantum dots with strong Coulomb interaction between elementary cells. In addition, we consider the effect of an external magnetic field and show that it results in stabilization of ordering in an electron system.

2. The model

We consider two-dimensional (2D) periodical structures of paired quantum dots ('molecules') depicted in figure 1(a) (triangular lattice) and figure 1(b) (square lattice). Within each molecule the electrons move in the double-well potential. We neglect the tunnelling between different molecules and suppose the intramolecular tunnelling (between the neighbouring dots) to be sufficiently small. This allows us to use the tight-binding approximation for calculating the molecular wave function. We suppose that there is only one electron per an elementary cell and take into account the Coulomb interaction between

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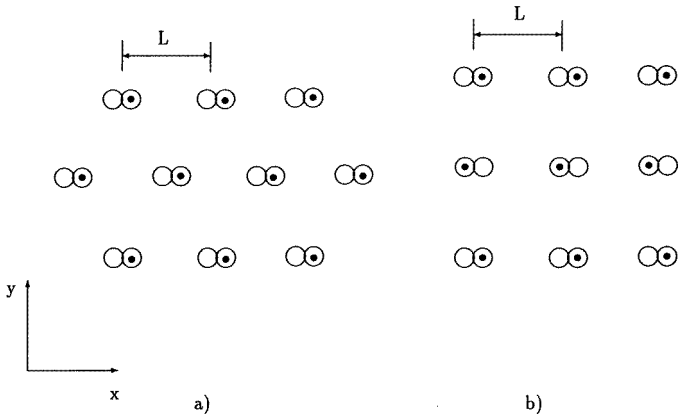

Figure 1. Molecular-like lattices of quantum dots: (a) the triangular lattice with ferroelectric arrangement; (b) the square lattice with antiferroelectric arrangement.

'molecules'. Coulomb interaction will be treated in the dipole–dipole approximation, which is valid in the limit $L \gg d$, where L is the lattice period and d is the distance between dots in a molecule. It was shown in our previous paper [4] that the ground states of triangular and square lattices of paired quantum dots are ferroelectric and antiferroelectric, respectively (figure 1).

The Coulomb interaction between molecules creates an electrostatic electric field $\boldsymbol{F}^{int}(\boldsymbol{r})$ that can lead to the electron polarization of molecules. In the tight-binding approximation, the dipole moment of a molecule in the lattice site α is straightforwardly derived on the basis of a two-level model:

$$P_{\alpha x} = e\langle x_\alpha \rangle = \frac{ed}{2}\frac{\Delta_\alpha}{\sqrt{\Delta_\alpha^2 + 4V^2}}\tanh\frac{\delta E_\alpha}{2T} \qquad \Delta_\alpha = ed\,F_x^{int}(\boldsymbol{R}_\alpha) \tag{1}$$

where $\boldsymbol{r} = (x, y)$ is the 2D radius vector, $\boldsymbol{e}_x$ is the molecular axis, $\boldsymbol{R}_\alpha$ is the lattice vector corresponding to the centre of the α-molecule, $x_\alpha = x - R_{\alpha x}$, V is the tunnelling amplitude, $\delta E_\alpha = \sqrt{4V^2 + \Delta_\alpha^2}$, T is temperature, and $\hbar$ is assumed to be unity.

The absolute value of the spontaneous electric field for ferroelectric (antiferroelectric) states in corresponding lattices (figure 1) at any lattice site is

$$F_x^{int} = C_i\frac{ed\,P_x}{\epsilon L^3} \tag{2}$$

where the index i can be tr and sq for triangular and square lattices, correspondingly, $C_{tr} = 5.5$ and $C_{sq} = 5.1$, and ϵ is the background dielectric constant. The spontaneous electric moment is determined by the equation

$$\gamma C_i\frac{2}{\sqrt{\Delta^2/V^2 + 4}}\tanh\frac{\delta E}{2T} = 1 \tag{3}$$

where $\gamma = e^2d^2/(4VL^3\epsilon)$. A nontrivial solution of this equation exists if $C_i\gamma\tanh V/T > 1$. The phase transition temperature is given by

$$T_0 = 2V\Big/\ln\left(\frac{\gamma C_i + 1}{\gamma C_i - 1}\right) \tag{4}$$

(see, e.g., [5]). We now estimate the temperature of the phase transition for the lattice of GaAs quantum dots with parameters $L = 700$ Å, $d = 200$ Å and $\epsilon = 13$. Using equation (4) we have $T_0 \simeq 2$ K in the limit of small tunnelling amplitudes $V \ll C_i e^2 d^2/(4\epsilon L^3)$, when $T_0 \simeq C_i e^2 d^2/(4\epsilon L^3)$.

3. The spectrum of collective excitations

Our next goal is the response function of the quantum dot lattice. If $\boldsymbol{f}_0 \exp(-\mathrm{i}\omega t + \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r})$ is the external electric field, the effective field at each lattice site is $\boldsymbol{f}_0 + \boldsymbol{f}_{ind}$, where $\boldsymbol{f}_{ind}$ takes into account the contribution of surrounding cells. In the self-consistent-field approximation the field $\boldsymbol{f}_{ind}$ is expressed via the dipole moments of elementary cells. It is convenient to use the Fourier transformation

$$P_x^{ind}(\boldsymbol{q},\omega) = \sum_\alpha \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_\alpha} P_{\alpha x}^{ind} \tag{5}$$

where $P_{\alpha x}^{ind}$ is the moment induced by the external electric field in the α-molecule. Using the linear-response theory we find the induced dipole moment

$$\begin{aligned} P_x^{ind}(\boldsymbol{q},\boldsymbol{\omega}) &= -\frac{\kappa}{\omega^2 - \omega_i^2(\boldsymbol{q})} f_{0x} \\ \kappa &= e^2 d^2 \frac{2V^2 \tanh(\delta E/2T)}{\sqrt{\Delta^2 + 4V^2}} \end{aligned} \tag{6}$$

where the frequency of collective excitations is

$$\omega_i^2(\boldsymbol{q}) = 4V^2 + \Delta^2 - \gamma \frac{8V^3 \tanh(\delta E/2T)}{\sqrt{\Delta^2 + 4V^2}} s_i(\boldsymbol{q}). \tag{7}$$

The $\boldsymbol{q}$-dependence of the collective mode frequency ω_i is determined by the function

$$s_i(\boldsymbol{q}) = L^3 \sum_\alpha \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_\alpha} \frac{2R_{\alpha x}^2 - R_{\alpha y}^2}{R_\alpha^5}. \tag{8}$$

The dispersion for temperatures $T > T_0$ is written as

$$\omega_i^2(\boldsymbol{q}) = 4V^2 \left(1 - \gamma \tanh\left(\frac{V}{T}\right) s_i(\boldsymbol{q})\right) \tag{9}$$

where the second term is the so-called depolarization shift. In the regime of the phase transition $T < T_0$, we have to take into account a nonzero value of Δ in equation (7). Using equation (3), we may write the collective excitation dispersion in the regime of the phase transition in the form

$$\omega_i^2(\boldsymbol{q}) = 4V^2 \left(1 - \frac{s_i(\boldsymbol{q})}{C_i}\right) + \Delta^2. \tag{10}$$

Note that the function $s(\boldsymbol{q})$ has the following properties: $C_{tr} = s_{tr}(0)$, $C_{sq} = s_{sq}(\boldsymbol{e}_y \pi/L)$ and $C_i = \max(s_i(\boldsymbol{q}))$. Using these properties, one can see that $\omega_i^2(\boldsymbol{q}) \geqslant 0$ for any temperature. The latter confirms our choice of ground states for triangular and square lattices.

The character of the ordered phase can be understood by analysing the dispersion of collective excitations in a system. The dispersion laws of collective excitations in triangular and square lattices at the temperature T_0 (equation (4)) are shown in figures 2 and 3. In the molecular-like system only an x-component of the polarization vector is possible. This is why the modes with $\boldsymbol{q}||\boldsymbol{e}_x$ are longitudinal, while the modes with $\boldsymbol{q}||\boldsymbol{e}_y$ are transversal.

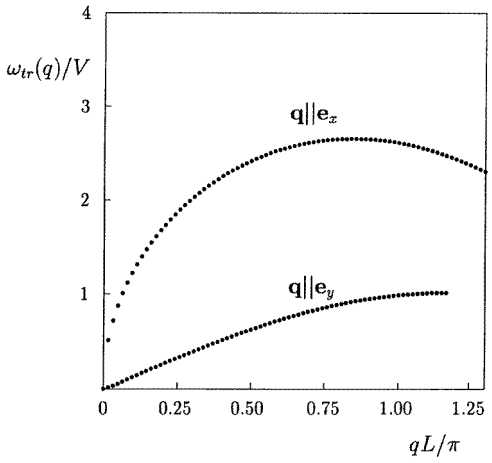

Figure 2. Dispersion of collective excitations in the triangular lattice at the temperature of the ferroelectric phase transition.

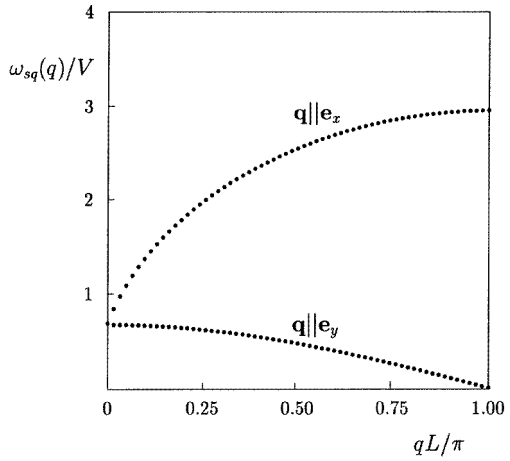

Figure 3. Dispersion of collective excitations in the square lattice at the temperature of the antiferroelectric phase transition.

One can see that the collective excitation frequency of the triangular lattice tends to zero for $\boldsymbol{q} \to 0$. In the case of the square lattice the momentum corresponding to zero frequency is $(\pi/L)\boldsymbol{e}_y$ and relates to the transversal mode. Thus, triangular and square lattices demonstrate ferroelectric and antiferroelectric phase transitions, respectively. In the vicinity of phase transitions, the frequencies at the critical points of dispersion are proportional to $\sqrt{|T - T_0|}$. It is interesting to study the dispersion of collective modes near the critical points at $T = T_0$. By using equation (7) and some properties of the function $s(\boldsymbol{q})$, we have for $T = T_0$

$$\begin{aligned} \omega_{tr}^2 &= a\frac{q_x^2}{q} + bq_y^2 \qquad q \simeq 0 \\ \omega_{sq}^2 &= a'q_x^2 + b'(q_y - \pi/L)^2 \qquad \boldsymbol{q} \simeq (0, \pi/L) \end{aligned} \tag{11}$$

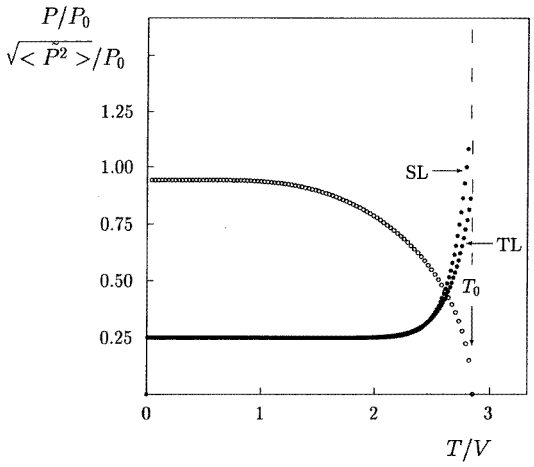

Figure 4. Spontaneous polarization P (open circles) and the amplitudes of quantum fluctuations $\sqrt{\tilde{P}^2}$ (closed circles) as functions of temperature for the triangular lattice (TL) and square lattice (SL) ($\gamma = 3$, $P_0 = ed/2$).

where a and b are constants. It is seen from equation (11) that the frequency of the triangular lattice ω_{tr} is not analytical near the critical point $q = 0$ and is proportional to $\sqrt{q}$ when $q_y L \ll q_x L \ll 1$. In the square lattice the frequency ω_{sq} shows acoustical-like behaviour near the boundary of the Brillouin zone.

4. Quantum fluctuations

In this section we calculate the correlation functions in an effort to understand the role of fluctuations in the presence of ferroelectric (antiferroelectric) ordering.

The quantum fluctuations in the system can be described by the correlation function $\langle\tilde{x}_\alpha^2\rangle$, where $\tilde{x}_\alpha = x_\alpha - \langle x_\alpha\rangle$. To find this function, we may use the fluctuation-dissipation theorem:

$$S(\boldsymbol{q},\omega) = \int \mathrm{e}^{\mathrm{i}\omega t}\langle\tilde{x}^*(\boldsymbol{q})\tilde{x}(\boldsymbol{q},t)\rangle\ \frac{\mathrm{d}t}{2\pi} = -\frac{n(\omega)+1}{\pi e^2}\,\mathrm{Im}F(\boldsymbol{q},\omega) \tag{12}$$

where the response function $F(\boldsymbol{q},\omega)$ can be written as $F(\boldsymbol{q},\omega) = \kappa/(\omega^2 - \omega_i^2)$ (see equation (6)). By using equation (12), we get the amplitude of fluctuations of the dipole moment $P = ex_\alpha$:

$$\langle\tilde{P}^2\rangle = \frac{1}{N}\sum_{\boldsymbol{q}}\frac{\kappa}{\omega_i(\boldsymbol{q})}\left(n(\omega_i)+\frac{1}{2}\right) \tag{13}$$

where N is the number of elementary cells in the 2D system.

We note that the mean squared fluctuation of the dipole moment (13) remains finite for any temperature excepting, possibly, the phase transition temperature T_0, because all frequencies $\omega_i(\boldsymbol{q})$ are nonzero for $T \neq T_0$. The latter distinguishes our system from a 2D Wigner crystal, where the acoustical-like mode destroys the long-range order of an electron lattice [6].

Numerical results for the T-dependence of the correlation function are shown in figure 4 for the parameter $\gamma C_i = 3$. If $\gamma C_i \gg 1$, the amplitude of fluctuations is much less than the

average spontaneous dipole momentum P in the temperature region $T_0 - T \simeq T_0$ and exceeds P in the near vicinity of the temperature of the phase transition when $(T_0 - T)/T_0 \simeq 1/(\gamma C_i)$. In the case where $\gamma C_i \gg 1$ and $T_0 - T \simeq T_0$, we may use the approximation

$$\sqrt{\langle \tilde{P}^2 \rangle}/P_0 = \frac{1}{\sqrt{2} C_i \gamma} = \frac{V}{\sqrt{2} C_i E_c} \tag{14}$$

where $P_0 = ed/2$ and $E_c = e^2 d^2/(4\epsilon L^3)$ is the characteristic energy of Coulomb interaction between elementary cells. One can see that the ratio $\sqrt{\langle \tilde{P}^2 \rangle}/P_0$ decreases on reducing the tunnelling amplitude and with increasing Coulomb interaction between elementary cells. Note that the constant C_i plays the role of the effective number of interacting elementary cells. The dependence $\sqrt{\langle \tilde{P}^2 \rangle} \propto 1/C_i$ is typical for fluctuations in ferroelectric crystals [5]. Thus, we may conclude that ferroelectric (antiferroelectric) phases are stable if $\gamma C_i \gg 1$ and the temperature is not too close to T_0.

For the parameter $C_i \gamma \gg 1$ the amplitude of fluctuations in the triangular lattice is close to that for the square lattice except in the near vicinity of the temperature T_0 (see figure 4). By using equations (11) and (13), one can show that the value of $\sqrt{\langle \tilde{P}^2 \rangle}/P_0$ in the triangular lattice remains finite even at $T = T_0$, while the same value in the square lattice becomes infinite in the limit $N \to \infty$: $\sqrt{\langle \tilde{P}^2 \rangle}/P_0 \propto \ln N$ when $T = T_0$. These facts are connected with different behaviours of the dispersion law (11) for triangular and square lattices.

5. The influence of the magnetic field

We now briefly consider the effect of high magnetic fields on phase transitions in a molecular-like array of quantum dots. It is known that the magnetic field may lead to stabilization of the electron Wigner crystals [6] and may suppress quantum fluctuations in quantum dots [7]. In [7], this fact has been demonstrated numerically for two anisotropic quantum dots. In our model, the magnetic field B has influence only on the tunnelling amplitude $V(B)$. We may expect that the tunnelling amplitude decreases with increasing magnetic field, because the magnetic field leads to additional localization of electrons. In high magnetic fields the tunnelling amplitude is expected to behave as: $V(B) \propto \exp(-d^2/2l_c^2)$, where l_c is the magnetic length. Just for a qualitative illustration of this statement let us consider the appropriate 1D model, in which the potential energy of 2D electrons depends only on x:

$$U(x) = -u_0[\delta(x - d/2) + \delta(x + d/2)] \qquad u_0 > 0. \tag{15}$$

The magnetic field $\boldsymbol{B}$ is parallel to the $0z$-direction. The exact solution of such a problem is expressed via the parabolic cylinder functions $D_p(\xi_k)$ and $D_p(-\xi_k)$, where ξ_k is the dimensionless coordinate of the Landau oscillator: $\xi_k = (x - l_c^2 k_y)/l_c$, k_y is the momentum in the y-direction, $p = E/\omega_c - 1/2$, and E is the energy. The dispersion equation for E is straightforward (we give it here only for $k_y = 0$):

$$D_p'(d/l_c) + D_p'(-d/l_c) = -\frac{u_0}{\omega_c}[D_p(-d/l_c) \pm D_p(d/l_c)] \tag{16}$$

where $D_p'(\xi) = \mathrm{d}D_p(\xi)/\mathrm{d}\xi$. For large magnetic fields, when $l_c \ll d$, we have to use the asymptotics of the function $D_p(\xi)$. Then one can see that two roots E_1, E_2 of the dispersion equation become closer to each other when B increases, in accordance with the formula $E_1 - E_2 \propto \exp(-d^2/2l_c^2)$. Thus, the magnetic field enlarges the polarizability of the molecular-like quantum dot that facilitates the phase transition.

Let us assume that the phase transition is not possible at zero magnetic field, i.e. $\gamma C_i \tanh(V/T) = (E_c/V)C_i \tanh(V/T) < 1$ for $B = 0$. On increasing the magnetic field we may satisfy the condition of the phase transition because of decreasing the tunnelling amplitude. Thus, the magnetic field is able to induce the phase transition. In the presence of ferroelectric (antiferroelectric) ordering the amplitude of fluctuations is proportional to V (see equation (14)) and, consequently, can be strongly suppressed in high magnetic fields.

6. Conclusions

We have calculated the spectrum of quantum fluctuations in a molecular-like array of quantum dots. The quantum fluctuations do not destroy ferroelectric (antiferroelectric) ordering if the energy of Coulomb interaction between elementary cells exceeds the tunnelling amplitude. It is shown that the external magnetic field can lead to a stabilization of ferroelectric (antiferroelectric) states.

Acknowledgments

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References

[1] Chaplik A V and Ioriatti L 1991 *Proc. 9th Int. Conf. on Electronic Properties of 2D Systems (Nara, Japan, 1991)* p 356; 1992 *Surf. Sci.* **263** 354
[2] Bakshi P, Broido D A and Kempa K 1991 *J. Appl. Phys.* **70** 5150
[3] Lent C S, Tougaw P D, Porod W and Bernstein G H 1993 *Nanotechnology* **4** 49
[4] Govorov A O and Chaplik A V 1994 *J. Phys.: Condens. Matter* **6** 6507
[5] Vaks V G 1973 *Introduction to the Theory of Ferroelectricity* (Moscow: Nauka) section III
[6] Ando T, Fowler A B and Stern F 1982 *Rev. Mod. Phys.* **54** 437
[7] Kempa K, Bakshi P, Broido D A and Blagoev K B 1994 *Solid State Commun.* **91** 231