Analogy Between Shape Transitions of a Quantum Dot in Magnetic Field and a Cranking Nucleus

Lucjan Jacak, Arkadiusz Wójs, and Władysława Nawrocka†

Institute of Physics, Technical University of Wrocław
Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland
†*Institute of Theoretical Physics, University of Wrocław*
Pl. M.Borna 9, 50-205 Wrocław, Poland

(Received 24 January 1996, accepted for publication 21 February 1996)

Shape dynamics of a system of two-dimensional electrons confined by an effective flexible potential is studied as a function of number of electrons, external magnetic field and temperature. Both in zero and non-zero magnetic field a spontaneous breakdown of the rotational symmetry of the system is identified for certain numbers of electrons. Oscillatory dependence of the system deformation on the number of electrons reflects filling of degenerate shells by electrons.

1. Introduction

Rapid progress in semiconductor technology has recently allowed creation of quasi-zero-dimensional structures, the so-called quantum dots or artificial atoms [1] and charging them with a well controlled number of electrons by applying a bias between the dot and a distant metal electrode [2]. Quantum dots are formed by imposing a lateral confinement to a quasi-two-dimensional electron gas. Since the confining potential is usually smooth, it can be very well approximated by a parabolic well [3, 4]. An important property of the parabolic potential is the single-particle energy spectrum consisting of equally spaced degenerate shells.

As shown in Refs.[5, 6] for a model of a nucleus, a system of non-interacting fermions confined to a three-dimensional parabolic well and only partially filling the valence shell, can under certain circumstances modify its self-consistent energy spectrum by changing its shape, i.e. spontaneously break the initially spherical symmetry of the confining potential. The shape phase transitions can also be induced by cranking of the nucleus, since cranking has a similar effect on the energy spectrum as a deformation (generates the anisotropy of single-particle modes) [5, 6].

One could expect a similar behavior of a parabolic quantum dot, where the number of particles (fermions) is of the same order of magnitude and the role of angular momentum in case of a cranking nucleus can be played by an external magnetic field. The main differences between the two systems are lower dimensionality in case of quantum dot and different nature of the interaction and confining potentials. The attractive short-range interaction between nucleons in a nucleus can be modeled by a smooth self-consistent single-particle field. While in general the electron-electron interaction in quantum dots cannot be neglected [4, 7] and the mean-field approach neglecting the electron-electron correlations is often unjustified [8], the interaction is relatively less important in very small dots (e.g. the self-assembled dots — SAD) where the kinetic energy quantization is the dominant effect [9].

We will show in the following that assuming hypothetically a freedom to adjust the (effective) confining potential leads to appearance of the magnetic field induced phase transitions of the quantum dot shape. In the light of the results for both systems studied here, a tendency to reorganize the energy spectrum by the system of non-interacting fermions partially filling the degenerate shell seems to be a general property, independent of the dimensionality.

Similar to Ref.[6] we shall adopt the thermodynamic approach, where the fixed parameters are temperature and the number of electrons, which corresponds to the considered physical situation. However, since the system contains only 10–100 electrons, we shall mainly concentrate on very low temperatures, where the thermodynamic potential governing the state of the system is equivalent to the ground state energy and including the temperature is merely a formal operation allowing for a convenient expression of the equations defining the state of the system in terms of the relevant derivatives.

2. Model

Let us consider a two-dimensional system of N spinless electrons in the x–y plane, confined by an effective lateral potential V, in an external magnetic field $\mathbf{B}$ along the z-axis. The confining potential V includes the rigid part V_R due to the discontinuity in the energy of the conduction band at the interface of the two materials forming the dot, external electric field produced by the electrode defining the dot etc., and the hypothetical flexible single-electron self-consistent field V_F, which can be attributed e.g. to the interaction with other confined electrons and/or the mobile positive background (valence-band holes) compensating the negative charge localized in the dot. The flexible contribution V_F gives the whole effective potential V a freedom to accommodate, on a limited scale, the energetically favorable shape for given external parameters.

Modeling for simplicity the potential V by an anisotropic parabolic well defined by two variational parameters (frequencies ω_x and ω_y), one can write the single-electron Hamiltonian in the form

$$\hat{H} = \frac{1}{2m}(\mathbf{p} - \frac{e}{c}\mathbf{A})^2 + \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2), \tag{1}$$

where m is the electron effective mass and $\mathbf{B} = \text{rot}\,\mathbf{A}$.

In analogy to the harmonic oscillator model of a nucleus [5, 6], the parameters ω_x and ω_y cannot be independent in order to model the cohesion and non-compressibility of the dot (preventing the electrons from spreading out or being squeezed to the point). Following this analogy we impose an additional constraint on ω_x and ω_y in the form of the conservation of the potential's volume:

$$\omega_x \omega_y = \omega_0^2 = \text{const}, \tag{2}$$

which is equivalent to choosing the potential's deformation $\alpha = \omega_x/\omega_y$ as the independent variational parameter. As will be seen later from Eq.(7), α measures directly the deformation of the dot shape.

After the diagonalization procedure, the Hamiltonian (1) attains the form of a pair of uncoupled harmonic oscillators with characteristic frequencies

$$\omega_\pm^2 = \frac{1}{2}(\omega_x^2 + \omega_y^2 + \omega_c^2) \pm \frac{1}{2}\sqrt{(\omega_x^2 - \omega_y^2)^2 + \omega_c^2(2\omega_x^2 + 2\omega_y^2 + \omega_c^2)}, \tag{3}$$

where $\omega_c = eB/mc$ is the cyclotron frequency. The single-electron energies are $\varepsilon_n = \hbar\omega_+(n_+ + \frac{1}{2}) + \hbar\omega_-(n_- + \frac{1}{2})$, where $n = [n_+, n_-]$.

We can now introduce the grand canonical ensemble. Grand canonical potential $\Omega(T, \mu, \omega_0, \omega_c)$ is expressed through the grand partition function $\mathcal{Z}$:

$$\Omega = -k_B T \ln \mathcal{Z} = -k_B T \sum_n \ln\left[1 + \exp\frac{\mu - \varepsilon_n}{k_B T}\right]. \tag{4}$$

As it is desirable to fix the average number of electrons instead of the chemical potential, we further introduce a new potential F via the following Legendre transformation:

$$F(T, N, \omega_0, \omega_c) = \Omega(T, \mu, \omega_0, \omega_c) + \mu N. \tag{5}$$

Thus we deal with four fixed parameters T, N, ω_0 and ω_c, and two independent internal variables α and μ. Assuming the system to be in equilibrium, we can define the necessary conditions for the minimum of potential F at given temperature, number of electrons and magnetic field:

$$\frac{\partial F}{\partial \mu} = 0, \qquad \frac{\partial F}{\partial \alpha} = 0, \tag{6}$$

which reduce to the form:

$$< 1 >= N \tag{7a}$$

$$< \overline{y^2} >= \alpha^2 < \overline{x^2} > . \tag{7b}$$

Here the bar denotes quantum average $\overline{(\ldots)}=< n|\ldots|n >$ in the single-electron state, and

$$< \ldots >= \sum_n \left[1 + \exp \frac{\varepsilon_n - \mu}{k_B T}\right]^{-1} (\ldots) \tag{8}$$

is the statistical averaging. Note that Eq.(7b) yields the geometrical interpretation of α as the parameter of shape deformation mentioned earlier. The equation set (7a,b) can be conveniently written in terms of thermodynamical averages over the quantum numbers $n_\pm$:

$$< 1 >= N, \tag{9a}$$

$$\left(< n_+ + \frac{1}{2} > \omega_+ - < n_- + \frac{1}{2} > \omega_-\right)(1 - \alpha) = 0. \tag{9b}$$

This set of two non-linear equations with respect to α and μ was solved numerically with a modified Newton's method.

There equation set (9a–b) has solutions of two types: symmetric (with $\alpha = 1$) and non-symmetric (with $\alpha \neq 1$). The symmetric solution can be found immediately by calculating the chemical potential μ from Eq.(9a) since Eq.(9b) vanishes in this case. For non-symmetric solutions both equations are important. Note, however, that the chemical potential μ and single-electron levels $\omega_\pm$ for non-symmetric solutions depend on magnetic field B only via frequencies $\omega_\pm$ given by Eq.(3). Therefore, whenever there is a non-symmetric solution for a field B_1 and certain values of μ and $\omega_\pm$, the solution for a different field B_2 can be constructed by changing α so that ω_+ and ω_- remain unchanged. Then, for unchanged μ, Eqs.(9) remain valid. These solutions cannot be constructed for arbitrarily high values of B_2 as required $\omega_\pm$ cannot be then obtained with any value of α. Hence, the dependence $\alpha(B)$ for the non-symmetric case can be obtained from the condition $d\omega_\pm/d\omega_c = 0$, which gives the equation

$$(\omega_x - \omega_y)^2 + \omega_c^2 = (\omega^*_{c,\nu})^2, \tag{10}$$

where $\omega^*_{c,\nu}$ is the critical value of ω_c above which the ν-th non-symmetric solution does not exist. Parameters $\omega^*_{c,\nu}$ (together with $\omega_\pm$ and μ) can be calculated e.g. through direct solution of Eqs.(9) for any B such that $\omega_c < \omega^*_{c,\nu}$ (e.g. for $B = 0$).

An interesting observation is that the fact that frequencies $\omega_\pm$, chemical potential μ, and consequently thermodynamical potential F do not depend on the magnetic field for a deformed configuration implies immediately that the system magnetization $M = \partial F/\partial B$ vanishes in this case.

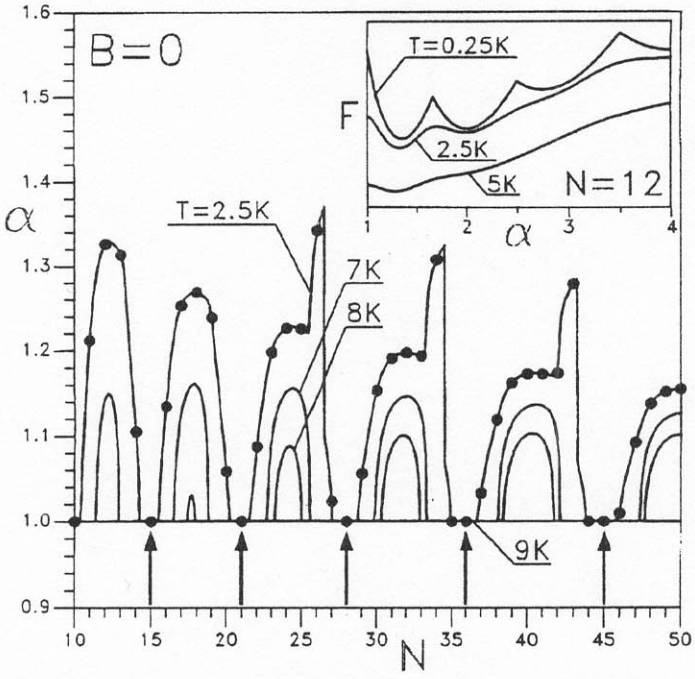

Figure 1. Dependence of the deformation parameter α on the average number of confined electrons N in zero magnetic field at different temperatures. Arrows indicate the 'magic' numbers: 15, 21, 28, 36 and 45. Inset: thermodynamic potential versus deformation parameter α.

3. Results

The scaling parameter ω_0 is the separation between single-electron energy levels in the symmetric case in zero magnetic field. For computations we assumed $\omega_0 = 2$ meV and the effective mass appropriate for GaAs, $m = 0.067\, m_e$. Presented results correspond to temperatures $T < 10$ K, at which the thermal spread $k_B T$ does not exceed half the excitation energy $\hbar\omega_0$.

Let us begin with description of the solutions in zero magnetic field. It was found that at sufficiently low temperatures ($T < 9$ K i.e. $k_B T < 0.4\hbar\omega_0$) the system was circular only within certain intervals of number of electrons N. Outside these intervals, in order to minimize their potential F, electrons spontaneously break the rotational symmetry and form an ellipse described by the deformation parameter α. The dependence of α on number of electrons N was examined and the resulting graphs for four different temperatures are presented in Fig.1. The inset shows the potential F as a function of α at fixed $N = 12$ (N determines the chemical potential through Eq.(9a)). It is clear that for this particular N potential F reaches its minimum at $\alpha \neq 1$. Although formally N is a continuous parameter here (a thermodynamic average), at very low temperatures, when the procedure of minimizing the potential F is equivalent to finding the system

ground state, the most important are configurations of integer N. They are marked in Fig.1 on the curve for $T = 2.5$ K with full circles.

Because of the shell structure of the energy spectrum, the low-temperature curves $\alpha(N)$ have a quasi-periodical character, with the period of several electrons. The intervals of circular symmetry narrow with decreasing T and eventually reduce to the 'magic' numbers in the limit $T \to 0$. The 'magic' numbers describe the configurations with completely filled shells. As for the two-dimensional parabolic potential the degeneracy of the shells grows linearly with the shell index, the series of 'magic' numbers $\mathcal{N}_k$ (indicated in Fig.1 with arrows) can be found immediately: $\mathcal{N}_k = \sum_{i=1}^{k} i = \frac{1}{2}k(k+1)$. For comparison, in the case of a three-dimensional parabola applicable e.g. to the nucleus [6] it is $\mathcal{N}_k^{3D} = \sum_{i=1}^{k} \frac{1}{2}i(i+1) = \frac{1}{6}k(k+1)(k+2)$. The chemical potential μ as a function of N exhibits sharp steps at the numbers $\mathcal{N}_k$ which therefore indeed indicate the stable configurations (excitation gap has a maximum and the fluctuation of N given by: $< N^2 > - < N >^2 = k_B T \, \partial N/\partial \mu$ drops down close to zero at $\mathcal{N}_k$).

When the temperature increases and the thermal spread $k_B T$ becomes comparable with the inter-shell separation $\hbar\omega_0$, the effect of the shell structure vanishes. The amplitude of oscillations of $\alpha(N)$ gradually decreases and above $T \approx 9$ K the oscillations decay completely – the shape is no longer sensitive to N. This process can be seen in the inset in Fig.1, where the deep minimum of F at $\alpha = 1.35$ is slowly pushed up with increasing T.

Let us now turn to the solutions in non-zero magnetic field B. In Fig.2 the thermodynamic potential F (solid lines) and deformation parameter α (dashed lines) have been plotted with respect to B for all solutions of the equation set (9). Number of electrons is $N = 12$ and temperature $T = 0.25$ K (for this temperature the curves differ very little from those for $T \to 0$). We have labeled the symmetric solution with the index 0 and all the non-symmetric (deformed) ones with indexes 1–5. Comparing curve (0) with the curve $F(\alpha)$ shown in the inset in Fig.1 one concludes the effect of applying an external magnetic field is very similar to that of the shape deformation. Indeed, according to Eq.3 both generate the anisotropy of single-electron modes ω_+ and ω_- which determines the ground state energy and the excitation gap of the system.

At sufficiently low temperatures the potential F_s of the symmetric state is not a monotonous function of B. The distinct parabolic-like parts of the curve $F_s(B)$ correspond to the configurations with different total angular momenta L. They are separated by the sharp peaks at the values of B when the well defined transitions between states with different L occur. The rising dependence $L(B)$ follows the magnetic field evolution of the two frequencies $\omega_\pm$, given by Eq.3. At $B = 0$ the degeneracy $\omega_+ = \omega_-$ implies $< n_+ >=< n_- >$ i.e. zero total

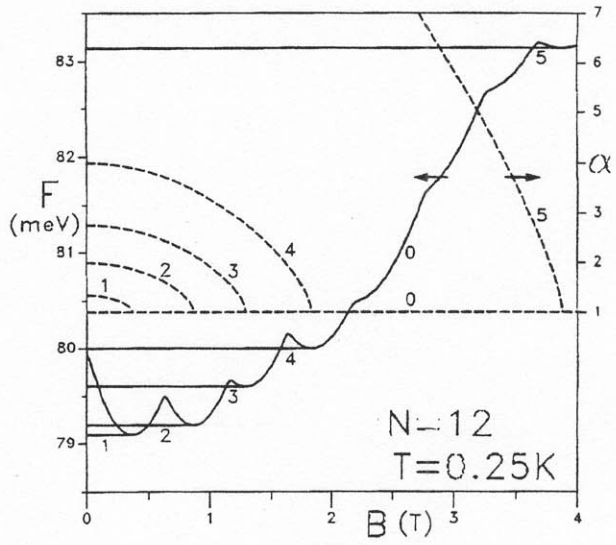

Figure 2. The complete set of solutions to Eqs.(9): thermodynamic potentials F (solid line) and deformation parameters α (dashed line), as functions of magnetic field B for $N = 12$ electrons at temperature $T = 0.25$ K. The symmetric solution (α=1) is labeled by 0 and deformed solutions are labeled by numbers 1–5.

angular momentum $L = \hbar < n_- - n_+ >$. When B increases this degeneracy is removed and successive electrons change their orbitals increasing L. Eventually in the strong fields B the structure of the Landau levels (LL) is formed and the two frequencies evolve into the intra-LL frequency: $\omega_- \to 0$, and the inter-LL frequency: $\omega_+ \to \omega_c$ (cf. Fig.3. Accordingly, in the lowest-energy configuration in this regime all electrons are restricted to the lowest LL: $< n_+ >= 0$.

It is seen from Fig.2 that in the regions of B when $\partial F_s/\partial B < 0$ the symmetric solution is thermodynamically unstable, i.e. it does not minimize the thermodynamic potential F. The analysis of equation set (9) reveals that a non-symmetric solutions appear, marked in Fig.2 as 1–5, with the constant potentials F_ν equal to the local minima of $F_s(B)$. According to Eq.10 these non-symmetric solutions exist only below the critical values of the field (i.e. of the cyclotron frequency $\omega^*_{c,\nu}$), that appear to be the values at which the potential F_s reaches its local minima F_ν:

$$\frac{\partial F_s}{\partial \omega^*_{c,\nu}} = 0. \tag{11}$$

Therefore, the pair of equations (10) and (11) allows for the calculation of all non-symmetric configurations, i.e. dependences $\alpha(B)$, $\mu(B)$ and $F(B)$, from the

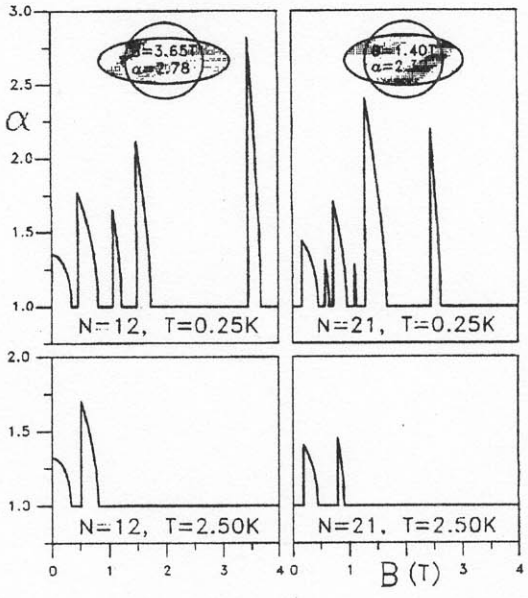

Figure 3. Magnetic field evolution of the deformation parameter α for the piece-wise continuous solutions of Eqs.(9) minimizing potential F. Each frame corresponds to the indicated number of electrons N and temperature T. Insets show the shapes of the extremally deformed dots.

dependence $F_s(B)$.

Behavior of the deformation parameter α_ν for each ν-th non-symmetric solution, following from Eqs.10 and 11, is also presented in Fig.2.

Increasing temperature leads to the appearance of the thermal mixing between different configurations. The dependence $L(B)$ evolves gradually from the step-like curve to a smooth line and so does the slope of the thermodynamical potential $(\partial F/\partial B)$. Consequently, the intervals of B where the non-symmetric solutions are favorable shrink and eventually disappear completely – the system is circular for all values of B. The thermal decay of the non-symmetric solutions is presented in Fig.3 where we show the field dependence of the deformation parameter α for two numbers of electrons $N = 12$ and 21 (deformed and symmetric shape in zero magnetic field, respectively) and two temperatures $T = 0.25$ K and $T = 2.5$ K (close to the zero-temperature limit and the intermediate regime, respectively). The field dependences of chemical potential μ, which together with α provide a complete solution of the equation set (9), is shown in Fig.4.

At each value of B we plotted α and μ corresponding to the thermodynamically stable solution, i.e. minimizing the potential F. As a result, the piece-wise continuous curves were obtained, showing discontinuous changes of the shape

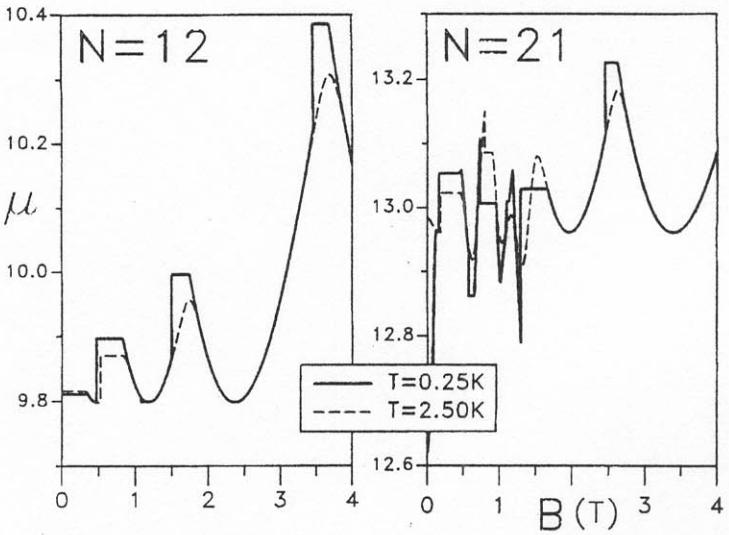

Figure 4. Magnetic field evolution of the chemical potential μ for the piece-wise continuous solutions of Eqs.(9) minimizing the potential F.

of the system, similar in all frames. An interesting observation is that the effect does not depend on whether the system was symmetric ($N = 12$) or not ($N = 21$) at $B = 0$. An increase in the number of electrons does not destroy the effect which persists for much larger N where the statistical approach becomes valid. It is also important to notice that the phase transitions from the symmetric to a deformed state are of the first order (thermodynamic potential F is not smooth and deformation parameter α is discontinuous) whereas the transitions from deformed to symmetric state – of the second order as only the slope of α is discontinuous.

The frequencies $\omega_{\pm}$ defined by Eq.3, independent of B for the non-symmetric configurations, define the single-electron excitation spectrum of the system. They can be measured directly as resonances by the far-infrared (FIR) spectroscopy methods.

In Fig.5 we plotted the evolution of the excitation spectra calculated for 12 and 21 electrons, at temperature $T = 0.25$ K ($k_B T = 0.01\hbar\omega_0$). The dashed lines indicate the symmetric-state curves (corresponding to the stable solutions at higher temperatures $T > 9$ K) are insensitive to the number of electrons N (the unique property of a harmonic well). The solid lines relate to the equilibrium solutions at low-temperature and contain the structure strongly dependent on N, reflecting the deformed configurations of the system.

Due to the so called generalized Kohn's theorem [7, 10] the electron-electron

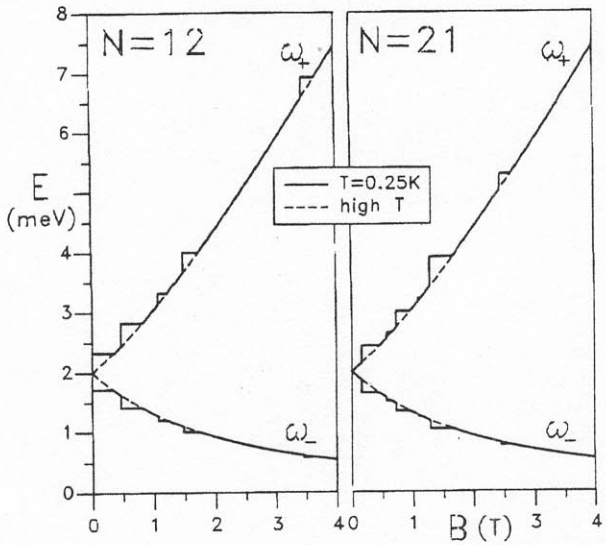

Figure 5. Magnetic field evolutions of the single-electron excitation spectra calculated for $N = 12$ and 21 electrons at temperature $T = 0.25$ K.

interaction, which is practically neglected within our model, does not influence the FIR spectrum of a rigid quantum dot as a consequence of the hidden symmetries associated with the parabolic confinement. In other words, in a real system the interaction does not introduce any deviations from the single-electron-like excitation spectrum and the effect of spontaneous deformation presented here should not be disturbed. In particular, removal of the $\omega_+ = \omega_-$ degeneracy at $B = 0$ for certain numbers of electrons at sufficiently low temperatures might be a useful test to verify our hypothesis.

However, the splitting between ω_+ and ω_- is fairly weak here (~ 0.6 meV for $N = 12$), so that this and all other energy-like parameters F, μ, $\omega_\pm$, ω_{xy}, characteristic temperatures, cyclotron frequencies (i.e. magnetic fields) etc. scale with the confining potential (ω_0). In very small dots (e.g. SAD), which can, however, contain fewer electrons, ω_0 can be larger by at least an order of magnitude significantly enhancing all the energies characteristic of the effect and increasing the critical temperatures.

In the above considerations we assumed that system was strictly two-dimensional. In the real quasi-two-dimensional quantum dots there is a potential pushing the electrons to the x–y plane, with the energy level separation in the z-direction much higher than ω_0. As a result, all electrons remain in the lowest level and the influence of excitations to higher levels is negligible. We have verified that including this effect only weakly modifies the dependence $\alpha(B)$ and the

shape transitions persist. An observable effect of the quasi-two-dimensionality, however insignificant in our model, is the finite spread of electrons wave-functions along the z-direction leading to the renormalization of the electron-electron interaction.

4. Conclusions

In summary, we have studied the shape dynamics of the system of quasi-two-dimensional non-interacting electrons confined by a parabolic well (quantum dot). The magnetic field induced phase transitions of the shape have been identified reflecting the tendency of the fermionic system partially filling the valence shell to reorganize its energy spectrum and lower the total energy. These phase transitions are analogous to those of a cranking nucleus.

It should be emphasized that the phase transitions identified here are due to the fermionic nature of electrons (or nucleons), which was taken into account by the minimization procedure for the system of particles occupying the available energy levels according to the Pauli exclusion principle, and described by an effective hamiltonian.

Described transitions have been obtained within the very simplified approach (one-particle approximation and equilibrium thermodynamics). Nevertheless, it would be extremely interesting to explore the possibility of their experimental realization since this effect might provide the basis for designing various electronic devices, for example a micro-switch controlled with magnetic field.

Acknowledgements

Two of us (L.J. and A.W.) wish to thank Pawel Hawrylak (IMS NRC, Ottawa, Canada) for useful comments and discussions.

References

[1] For the reviews and references see: M.Kastner, Physics Today, January 1993, page 24; T.Chakraborty, Comments in Cond. Matter Phys., 16 (1992) 35.

[2] R.Ashoori, H.L.Störmer, J.S.Weiner, L.N.Pfeiffer, K.W.Baldwin, K.W.West, Phys. Rev. Lett., 71 (1993) 613; H.Drexler, D.Leonard, W.Hansen, J.P.Kotthaus, P.M.Petroff, Phys. Rev. Lett., 73 (1994) 2252.

[3] A.Wójs, P.Hawrylak, S.Fafard, L.Jacak, to be published; A.Kumar, S.E.Laux, F.Stern, Phys. Rev., 42 (1990) 5166.

[4] P.Hawrylak, Phys. Rev. Lett., 71 (1993) 3347.

[5] A.Bohr, B.R.Mottelson, *Nuclear Structure, vol.II – Nuclear Deformations*, W.A.Benjamin, Inc. (1975); T.Troudet, R.Arvieu, Annals of Physics, 134 (1981) 1.

[6] L.Jacak, W.Nawrocka, R.G.Nazmitdinov, A.Wójs, J. Phys., G21 (1995) 1205.

[7] P.A.Maksym, T.Chakraborty, Phys. Rev. Lett., 65 (1990) 108.

[8] D.Pfannkuche, V.Gudmundsson, P.A.Maksym, Phys. Rev., B47 (1993) 2244; D.Pfannkuche, V.Gudmundsson, P.Hawrylak, R.R.Gerhards, Solid State Electronics, 37 (1994) 1221.

[9] P.M.Petroff, S.P.Denbaars, Superlattices and Microstructures, 15 (1994) 15.

[10] W.Kohn, Phys. Rev., 123 (1961) 1242; L.Brey, N.Johnson, B.Halperin, Phys. Rev., B40 (1989) 10647.