Control of Electronic and Optical Properties of Coupled Quantum Dots by Magnetic Field

N.E.Kaputkina* and Yu.E.Lozovik#

*Phys.Chem.Dept, Moscow State Institute for Steel and Alloys

#Institute of Spectroscopy, Academy of Sciences of Russia

- Single QD and QD systems
  - Horizontal QD molecules
  - Vertical QD molecules
- Singulet-triplet transition in CQD
- Strong electron correlation
- Quantum 'Crystallization'
- External magnetic field influence

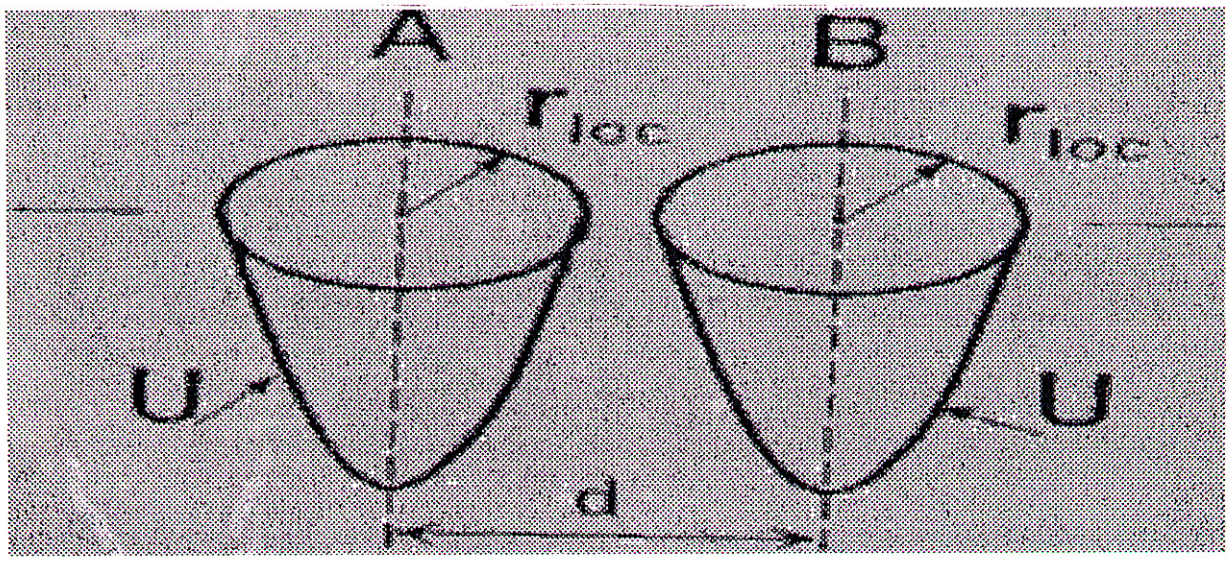
[1] PHYS. REV. LETT., 62, p.2164-2167 (1989)

QD molecule

Horizontal

Vertical

Horizontal QD molecule



Vertical QD molecule

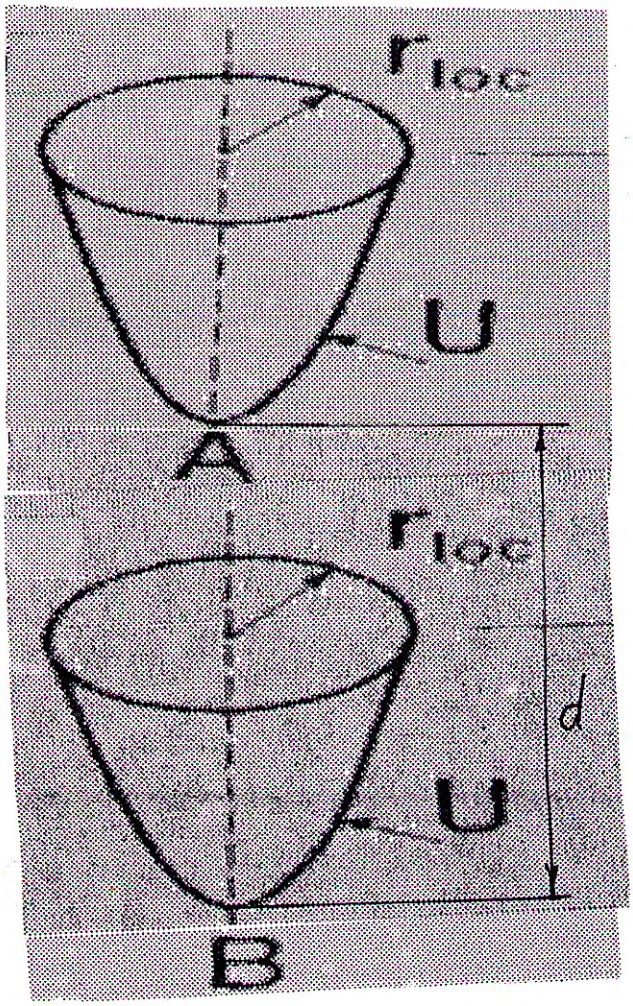
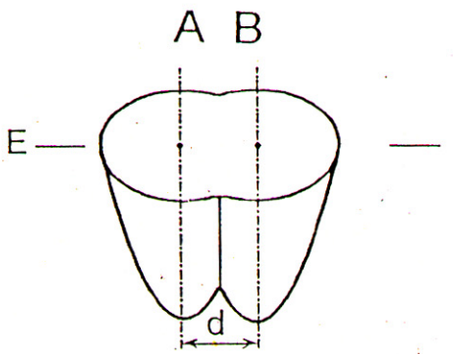
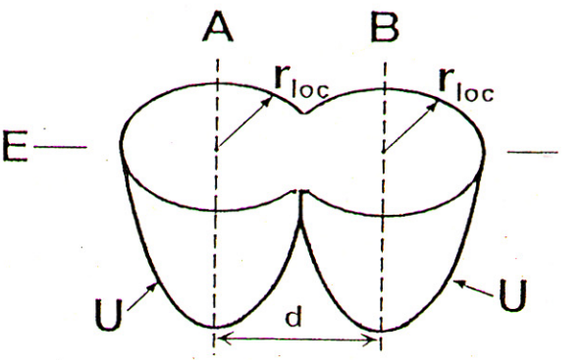
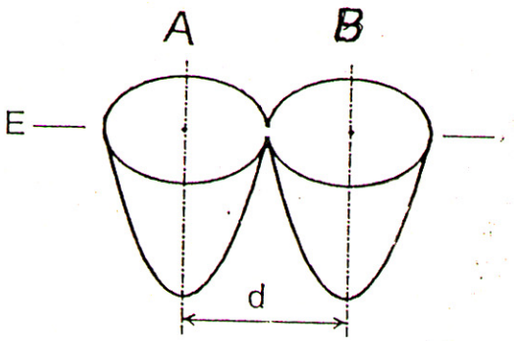


Fig.1 Horizontal QD molecule evolution; different approximation applicability

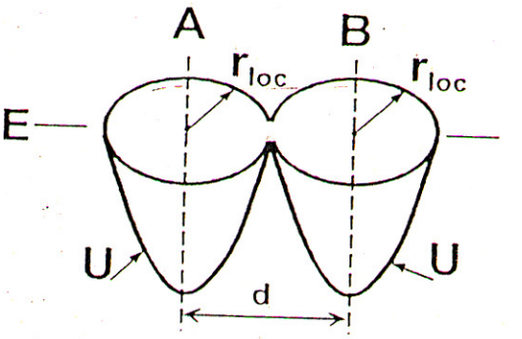


$d < r_{loc}$
a)Molecular orbital approximation
b)Variational method

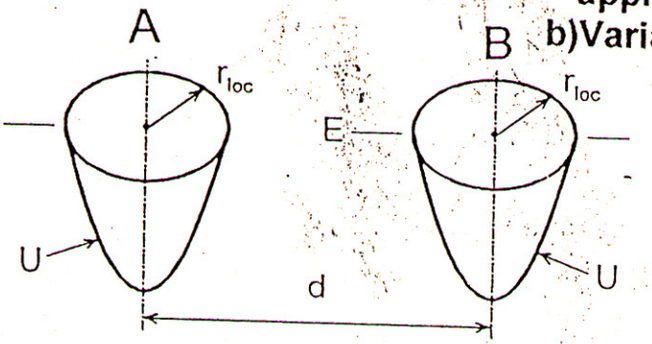


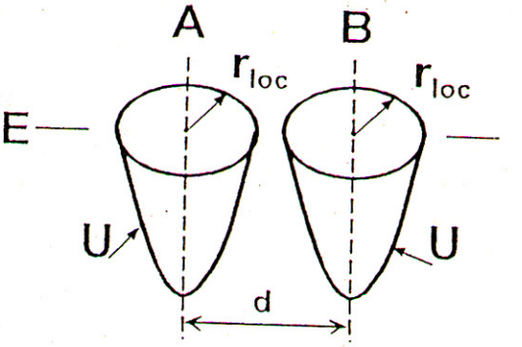


$d \sim r_{loc}$
b)Variational method



$d > k\, r_{loc}$ (k~3)
c)Heitler-London approximation
b)Variational method





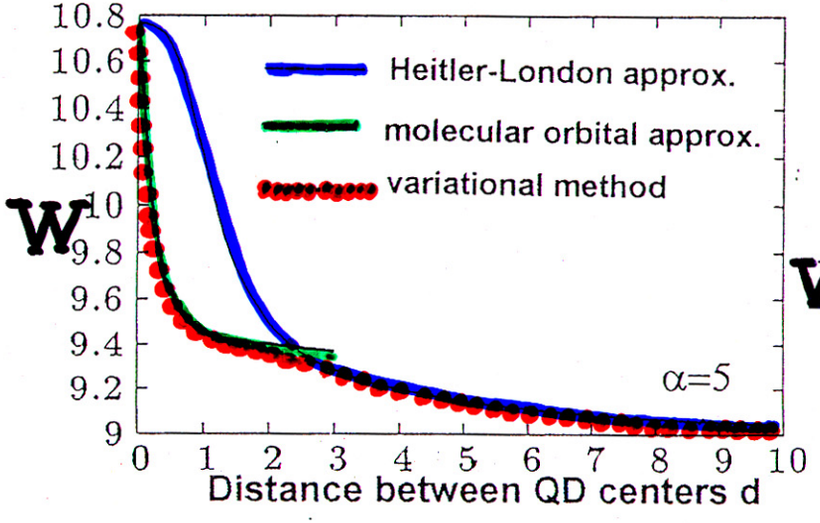
I with growth of distance between QD centers d at α=const

II with growth of confining potential steepness (effective steepness β^2 in external magnetic field) at d=const

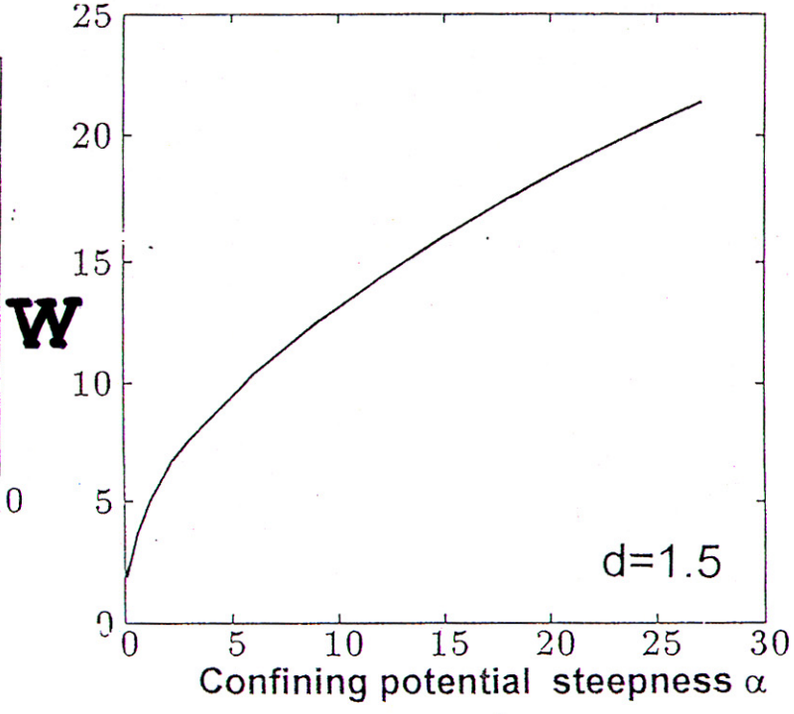
Ground state energy **W** of horizontal QD molecule

a) *versus* distance between QD centers d

b) versus the parameter of confining potential steepness α



a)



b)

$U = \alpha \min(r_A, r_B)^2$ – confining potential

a) Molecular orbital approximation

$$W = 2\varepsilon_0 + I_1 + I_2,$$

when $\varepsilon_0 = 2\sqrt{\alpha} + \frac{\alpha d^2}{2(1+e^{-\sqrt{\alpha}d^2/4})}$,

$I_1 = -\frac{d\alpha^2\Phi(\alpha^{1/4}d/2)}{2(1+e^{-\sqrt{\alpha}d^2/4})} - \frac{d\alpha^{3/4}}{\sqrt{\pi}}\frac{2e^{-\sqrt{\alpha}d^2/4}}{1+e^{-\sqrt{\alpha}d^2/4}}$;

$I_2 = \int\int \Psi^*_{mo}\frac{1}{r_{12}}\Psi_{mo}d\tau_1 d$;

$\Phi(x)$ – error function

$$\psi_{mo}(r) = \frac{1}{2(1+e^{-\sqrt{\alpha}d^2/4})}\left(\frac{\sqrt{\alpha}}{\pi}\right)^{1/2}\left(e^{-\sqrt{\alpha}r_a^2/2} + e^{-\sqrt{\alpha}r_b^2/2}\right)$$

b)Variational method

$$\psi_0(r) = \frac{\gamma}{\pi}e^{-\gamma r^2/2},$$

γ - variational parameter

c)Heitler-London approximation

$$W = 4\sqrt{\alpha} + \frac{1}{(1+e^{-\sqrt{\alpha}d^2})}(Q_к + J_к),$$

when $Q_к = \frac{\sqrt{\alpha}}{\pi}\int\int \frac{e^{-\sqrt{\alpha}(r_{1a}^2+r_{2b}^2)/2}}{r_{12}}d\tau_1 d\tau_2$

$J_к = \sqrt{(\pi/2)}\alpha^{1/4}e^{-\sqrt{\alpha}d^2}$.

$$\Psi = A[\psi_a(r_1)\psi_b(r_2) + \psi_a(r_2)\psi_b(r_1)]\xi_A(s_1, s_2)$$

when $\xi_A(s_1, s_2)$ - anti-symmetric spin function.

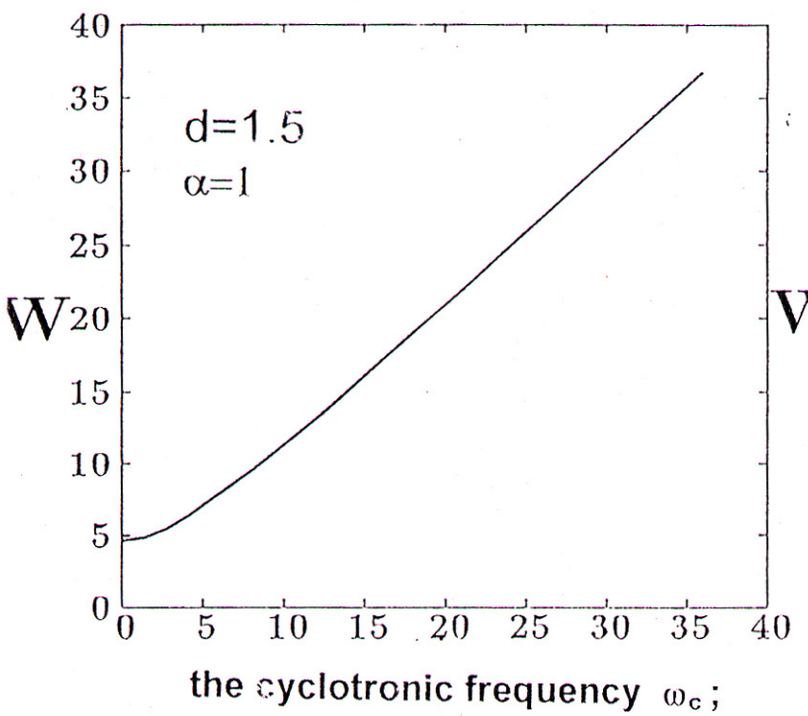
$\psi_a(r)$ и $\psi_b(r)$ – inperturbated wave functions of single QD

$\psi_{a,b}(r) = \left(\frac{\sqrt{\alpha}}{\pi}\right)^{1/2}e^{-\sqrt{\alpha}r_{a,b}^2/2}$.

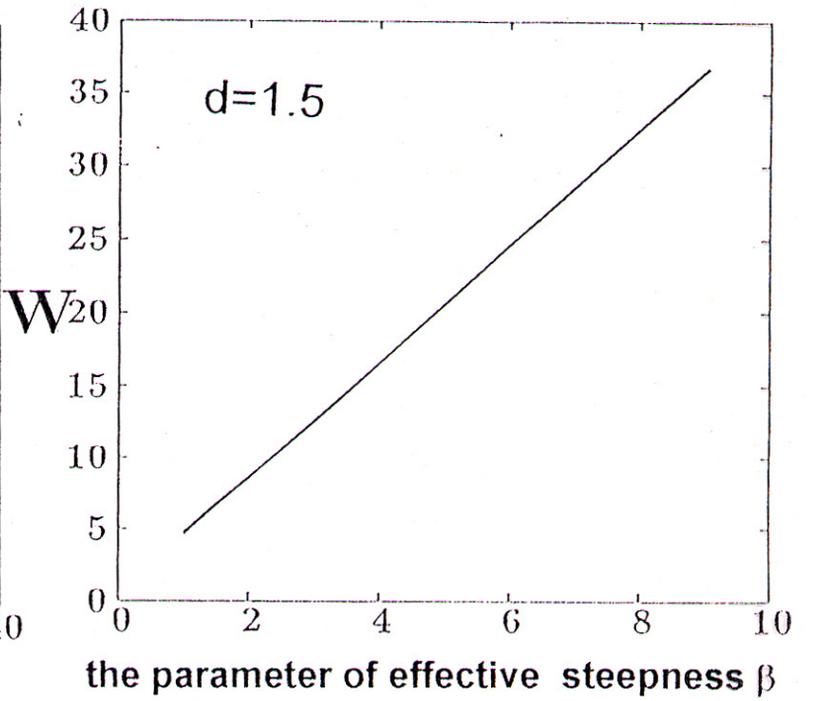
Ground state energy W of horizontal QD molecule in magnetic field

a) *versus* cyclotronic frequency ω_c ;

b) *versus* parameter of effective steepness of confining potential in magnetic field β



a)



b)

Van der Waals interaction energy E_v *versus* cyclotronic frequency ω_c

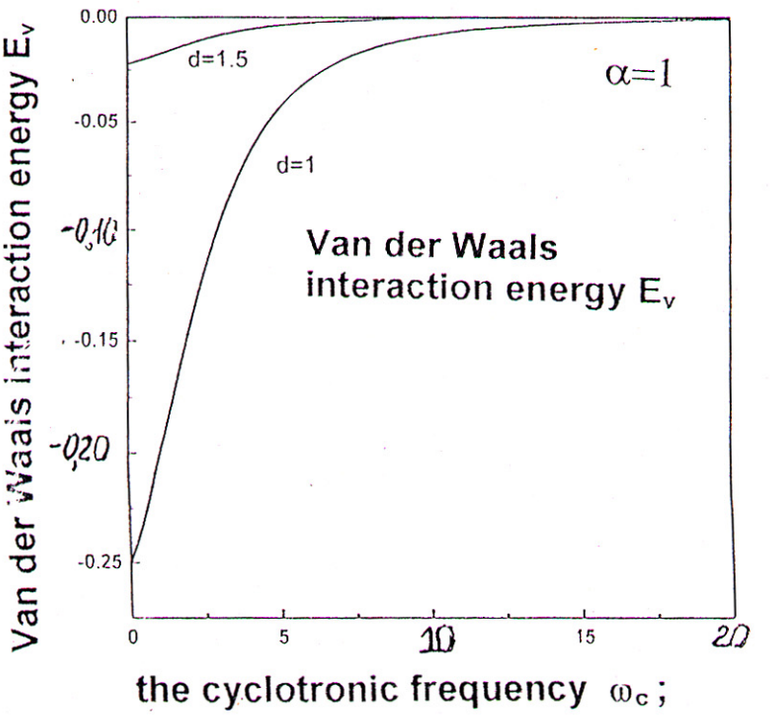
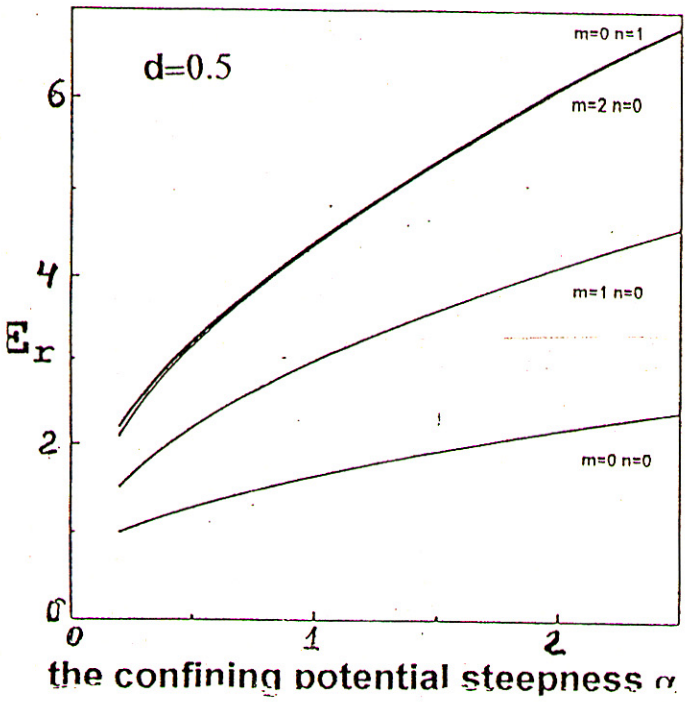


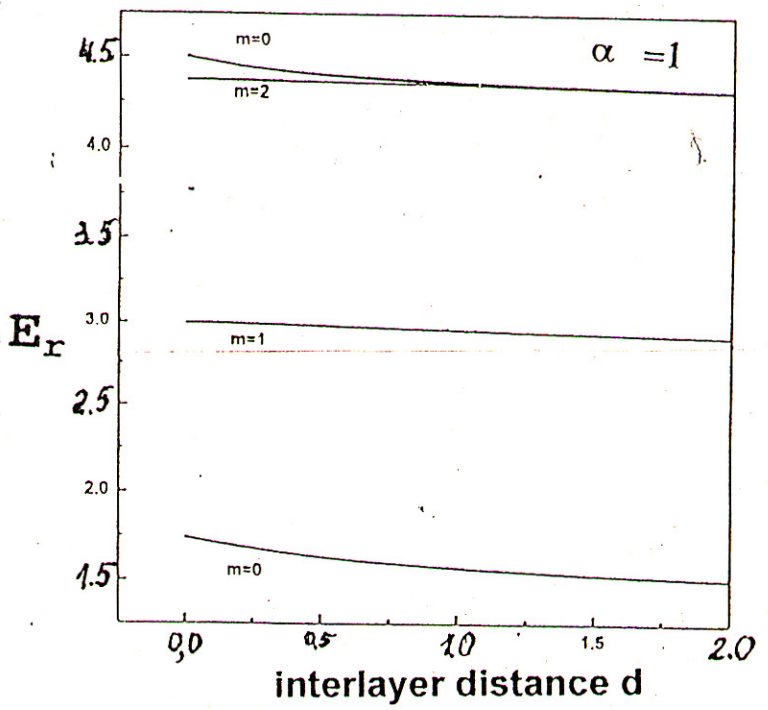
Fig.2. The dependencies of low-lying levels of electron relative motion energy E_r

a) *versus* the confining potential steepness α

b) *versus* interlayer distance d

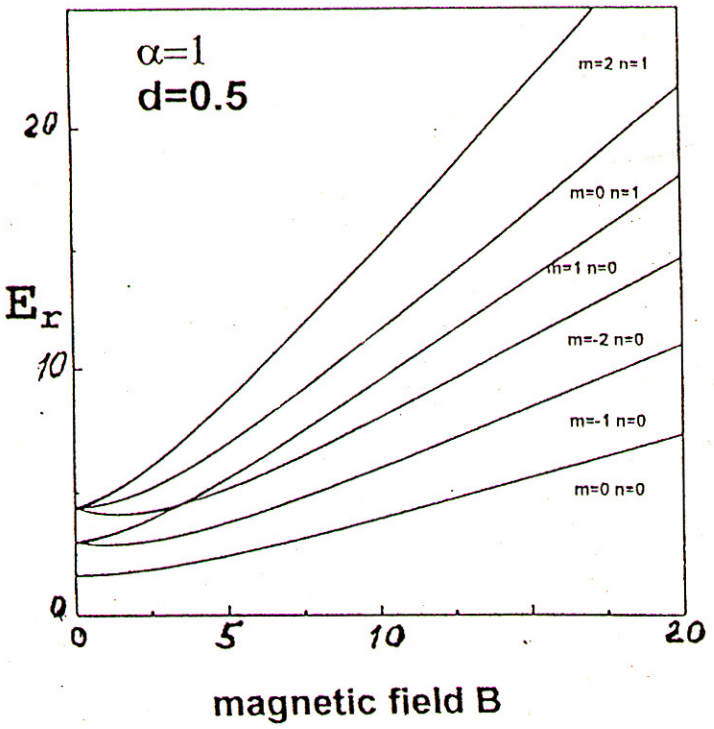


a)



b)

Fig.3. Magnetic field Influence on low-lying levels of electron relative motion energy E_r



1. $\hat{H} = \hat{H}_0 + \hat{H}_m$

$$\hat{H}_m = \frac{e}{2c}\left(\frac{A_1^2}{m_e^*} - 2\frac{i\hbar\nabla_1 A_1}{m_e^*} + \frac{A_2^2}{m_e^*} - 2\frac{i\hbar\nabla_2 A_2}{m_e^*}\right).$$

2. $\alpha \to \alpha' = \alpha + \omega_c^2/16$

3. $\varepsilon'_{nm} = \varepsilon_{nm} + m\omega_c/4.$

4. When $B \to \infty$,

$E_r \to 4\sqrt{\alpha'/2}(2n + |m| + 1) + \omega_c m/4.$

5. When $d \to \infty$,

$E \sim 2\sqrt{\alpha'/2}(2n + |m| + 1) + \omega_c m/4 +$
$+ 1/d - 1/(4\sqrt{\alpha'/2}d^3).$

6. When $d \to 0$ – The case of a single two-electron quantum dc

Vertical QD molecule

SINGULET-TRIPLET TRANSITION

Heitler-London approximation

Singulet state wave function

$$\Psi = A[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)]\xi_A(s_1, s_2) \qquad (1)$$

with $\xi_A(s_1, s_2)$ being anti-symmetric spin function.

Ground state energy

$$W_{sing} = 4\sqrt{\alpha} + \frac{1}{(1 + e^{-\sqrt{\alpha}d^2})}(Q_k + J_k), \qquad (2)$$

where $Q_k = \frac{\sqrt{\alpha}}{\pi}\int\int \frac{e^{-\sqrt{\alpha}(r_{1a}^2+r_{2b}^2)/2}}{r_{12}} d\tau_1 d\tau_2$

$J_k = \frac{\sqrt{\alpha}}{\pi}\int\int \frac{e^{-\sqrt{\alpha}/2(r_{1a}^2+r_{2b}^2+r_{1b}^2+r_{2a}^2)/2}}{r_{12}} d\tau_1 d\tau_2 = \sqrt{(\pi/2)}\alpha^{1/4}e^{-\sqrt{\alpha}d^2}$

Triplet state wave function:

$$\Psi = A[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) - \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)]\xi_A(s_1, s_2) \qquad (3)$$

Triplet state energy

$$W_{tripl} = 4\sqrt{\alpha} + \frac{1}{(1 - e^{-\sqrt{\alpha}d^2})}(Q - J), \qquad (4)$$

Triplet state occurs to be ground state if

$$\delta E_{tripl} - \delta E_{singl} = 2\frac{Qe^{-\sqrt{\alpha}d^2} - J}{(1 - e^{-2\sqrt{\alpha}d^2})} < 0, \qquad (5)$$

So singulet-triplet transition is possible in coupled QDs even in the absence of magnetic field !

MAGNETIC FIELD INFLUENCE

Parallel magnetic field controls spin state of QD system by change of the barrier between QDs

Transverse magnetic field influence comes to increase of confining potential steepness. Effective steepness of confining potential in magnetic field is $\beta^2 = \alpha + (\frac{\omega_c}{4})^2$.

Unperturbated wave functions of single-electron isolated QD in magnetic field

$$\psi_a(\mathbf{r}) = \psi_b(\mathbf{r}) = (\frac{\beta}{\pi})^{1/2} e^{-\beta r^2/2} \qquad (1)$$

$$W_{sing} = 4\beta + \frac{Q + J}{(1 + e^{-\beta d^2})}, \qquad (2)$$

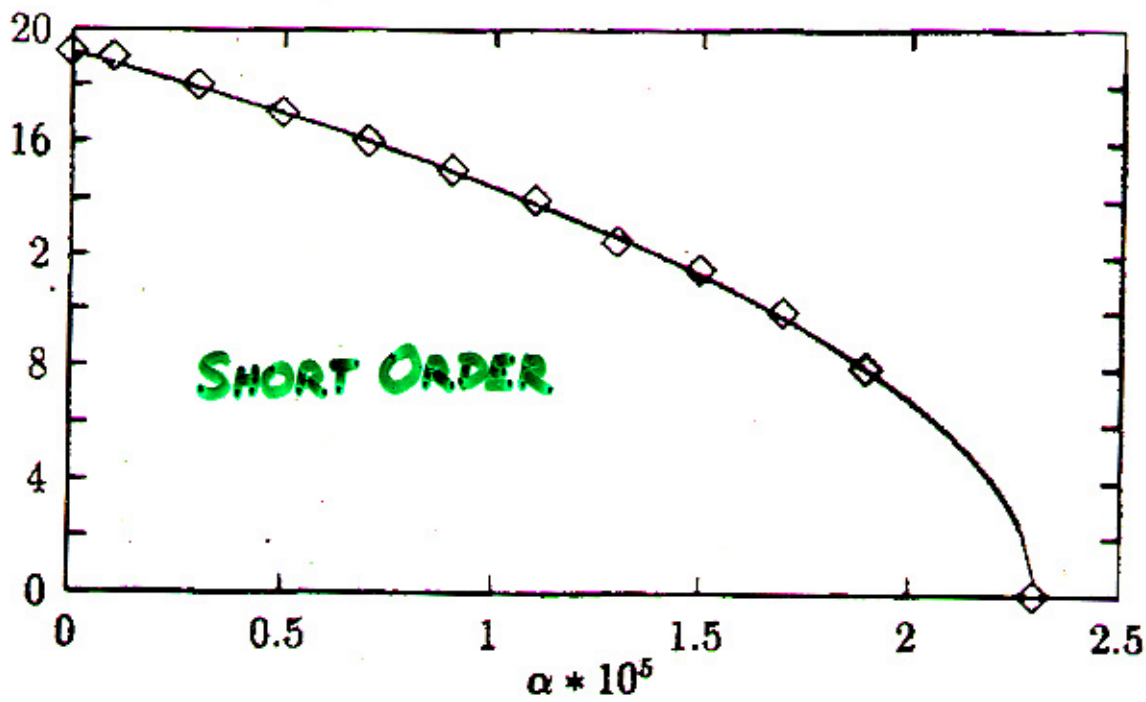
$$W_{tripl} = 4\beta + \frac{Q - J}{(1 - e^{-\beta d^2})}. \qquad (3)$$

With growth of magnetic field triplet state becomes the ground state of the QD system.

It is possible to control spin state of the QD system by external transverse magnetic field as well as by parallel magnetic field or by gate voltage.

'Crystallization' of 2D electron system

- **Classical regime:** dimensionless parameter $\Gamma^{class} = \frac{e^2}{ak_BT}$, $a = \frac{1}{(\pi n)^{1/2}}$ (n is two-dimensional density, k_B - Boltzman constant, T is temperature).
  Critical value for crystallization: $\Gamma^{class}_{cr} \sim 130$ corresponds to quasi-long-order state in Coulomb system (physical experiment for electron on He, computer simulations).
  Even at $T >> T_{melting}$ short-order survives. The last disappear at $\Gamma^{class}_{so} \sim 7$ (computer simulations by molecular dynamics).
- **Quantum regime:** dimensionless parameter $\Gamma^{quant} = \frac{e^2/r}{\hbar^2/mr^2} = \frac{r}{a_0} = r_s$ ($a_0 = \frac{\hbar^2}{m^* e^2}$ is effective Bohr radius, r = (πn)-1/2 is mean radius of circle occupied by one electron).
  Critical value for crystallization: at $T = 0$ $\Gamma^{quant}_{cr} = r_s^{cr} = 37$ corresponds to long-order state in Coulomb system (quantum Monte-Carlo).
  Assume that short order appears at $r_s^{so} \sim 3$. Lindeman parameter is $\Upsilon = \frac{\langle r^2 \rangle}{a_0^2} = r_s^{-3/2}$, $\langle r^2 \rangle$ is root-mean-squared electron deviation from wave function localization center. At $r_s \sim 3$ $\Upsilon_{so} \sim 3^{3/2} \sim 0.2$.



The schematic boundary (crossover) of electron quantum 'crystallization' region.

$$\gamma_{so} = 1/4 \quad \beta_{crit} = 0.005$$

The parabolic lateral confining potential $U(r) = \alpha r^2$

Numerical calculations with basis

l) single-particle eigenfunctions in confining potential

$$f_{nm} = \left(\frac{n!}{\pi(|m| + n)!} \left(\frac{\beta}{\sqrt{2}}\right)^{|m|+1} \right)^{1/2} r^{|m|} e^{-\left(\frac{\beta}{\sqrt{2}}\right) r^2/2} L_n^{|m|}\left(\frac{\beta}{\sqrt{2}} r^2\right) \quad (1)$$

2) harmonic oscillator eigenfunction with centers at centers of localization of electron

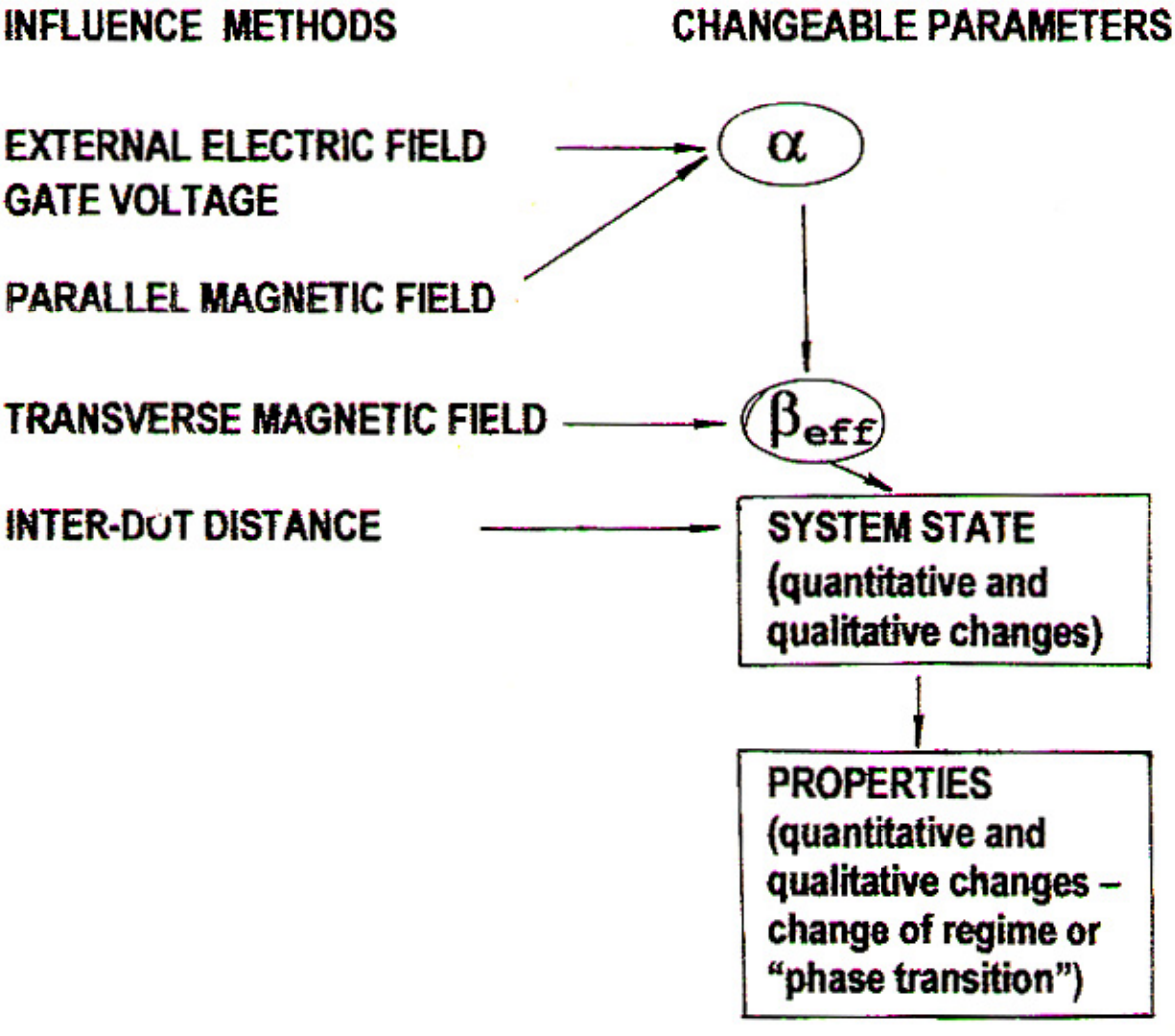
$$f_{nm}(x) = \left(\frac{1}{2^n n!}\sqrt{\frac{\sqrt{a_m/2}}{\pi}}\right)^{1/2} e^{-\frac{1}{2}\sqrt{\frac{a_m}{2}} x^2} H_n\left(\left(\frac{a_m}{2}\right)^{1/4} x\right) \quad (2)$$

$x = r - r_0$, r_0 is the mean distance between electrons,

$a_m = \beta^2 + \frac{2}{r_0^3} + \frac{6m^2}{r_0^4}$. $\beta = \sqrt{\alpha + (\omega_c/4)^2}$ **is effective steepness of confining potential in magnetic field.**

$$f_m = \sum_n C_{nr.} f_{nm} \quad (3)$$

POSSIBILITY TO CONTROL THE STATE OF SINGLE AND COUPLED QUANTUM DOTS



Quantitative changes of system state ⇨ QUALITATIVE CHANGES:

-Strong correlation

-Merging and separation of individual QDs

-Spin states :singulet-triplet transition

-Tunneling through the inter-dot barrier, etc.

Conclusion

Single quantum dots and quantum dot systems (horizontally and vertically coupled) was studied analytically and numerically taking into account inter-particle interaction.

Magnetic field influence on these systems is investigated. It' s possible to control system by normal and parallel magnetic field application transforming strongly coupled quantum dots with common charge carriers to separate ones.

We investigate also possibility to control spin states for CQD by external magnetic field as well as by steepness of confining potential.

We have studied singulet-triplet transition in CQD in the absence of magnetic field controlled by inter-dot coupling

Quantum "crystallization" of electron in QDs subjected to an external magnetic field is considered.

Quantum dot spectrum evolution is followed from one-particle spectrum in confining potential weakly perturbed by inter-electron interaction to region of strong electron correlation.

Magnetic field effect on the crystal order in few-electron quantum dots is *not monotonous* due to the competition of two mechanisms: magnetic field localizing effect and compression of the whole system due to increase of effective steepness of confining potential.