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QUANTUM WELLS, DOTS, WIRES
AND SELF-ORGANIZING NANOSTRUCTURES
11 - 22 AUGUST 1997**

**"Addition spectra and shell filling in quantum dots:
the role of electron-electron interactions"**

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These are preliminary lecture notes, intended only for distribution to participants.

**Addition spectra and shell filling in quantum dots:
the role of electron-electron interactions**

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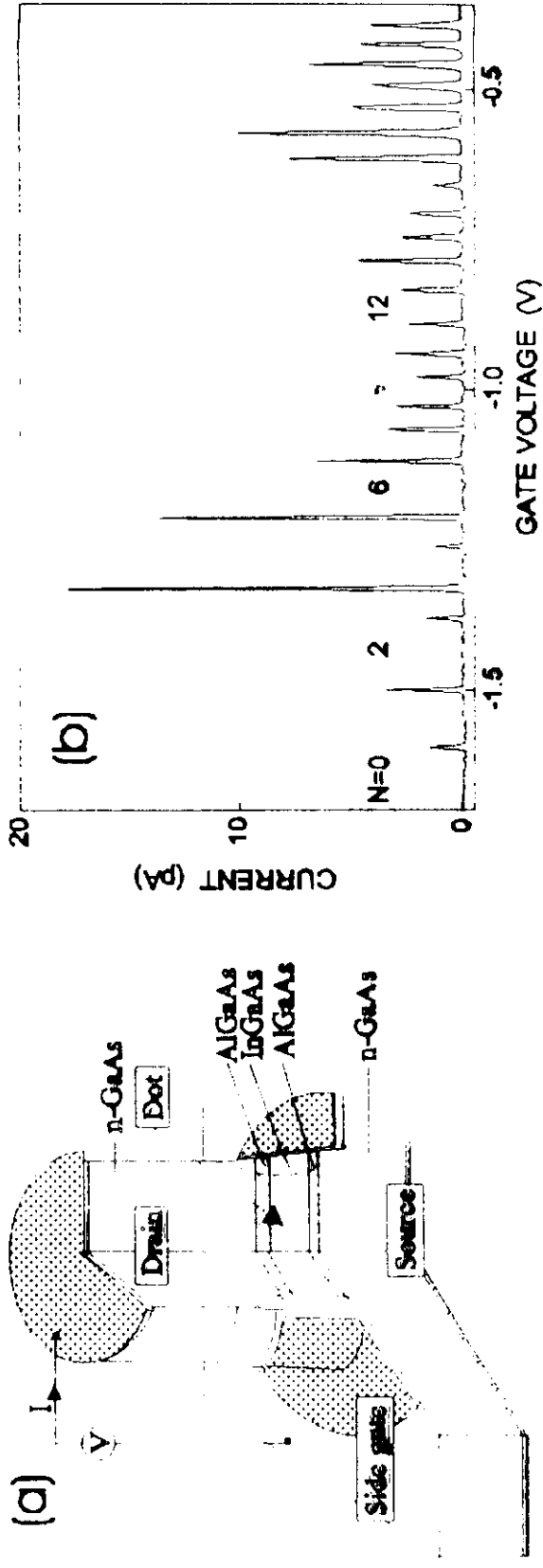


Figure 5.2. (a) Schematic diagram of the gated quantum dot device and (b) the Coulomb oscillations in the current vs. gate voltage at $B = 0$ T observed for a $0.5 \mu\text{m}$ diameter dot. (From Tarucha *et al.* [131].) (FROM TARUCHA *et al.*, PRL 77, 3673 (1996).)

WE CONSIDER ONLY VERTICAL QUANTUM DOTS
(QD) WITH HIGH SYMMETRY:

— PARABOLIC CONFINEMENT POTENTIAL WITH

CIRCULAR SYMMETRY $V(x, y) = \frac{1}{2} m^* \omega^2 r^2$

— SYMMETRIC WELL ALONG z AXIS

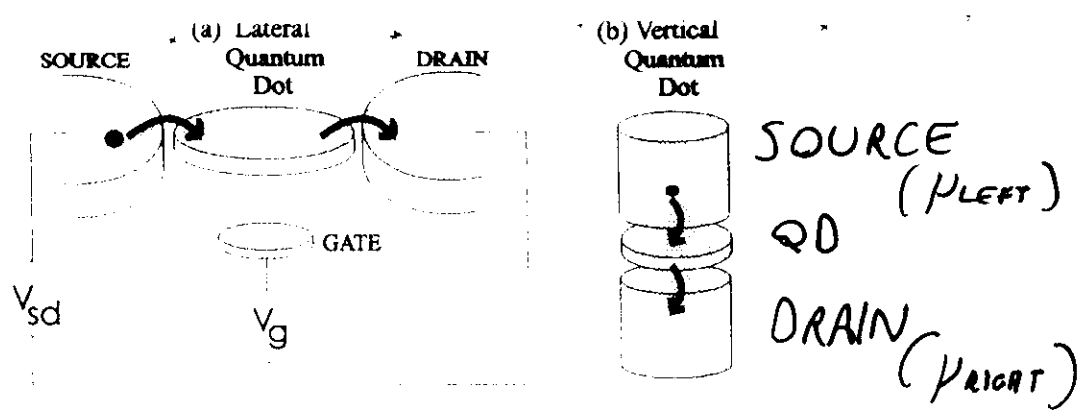


Figure 1.1. Schematic of a quantum dot, in the shape of a disk, connected to source and drain contacts by tunnel junctions and to a gate by a capacitor. (a) shows the lateral geometry and (b) the vertical geometry.

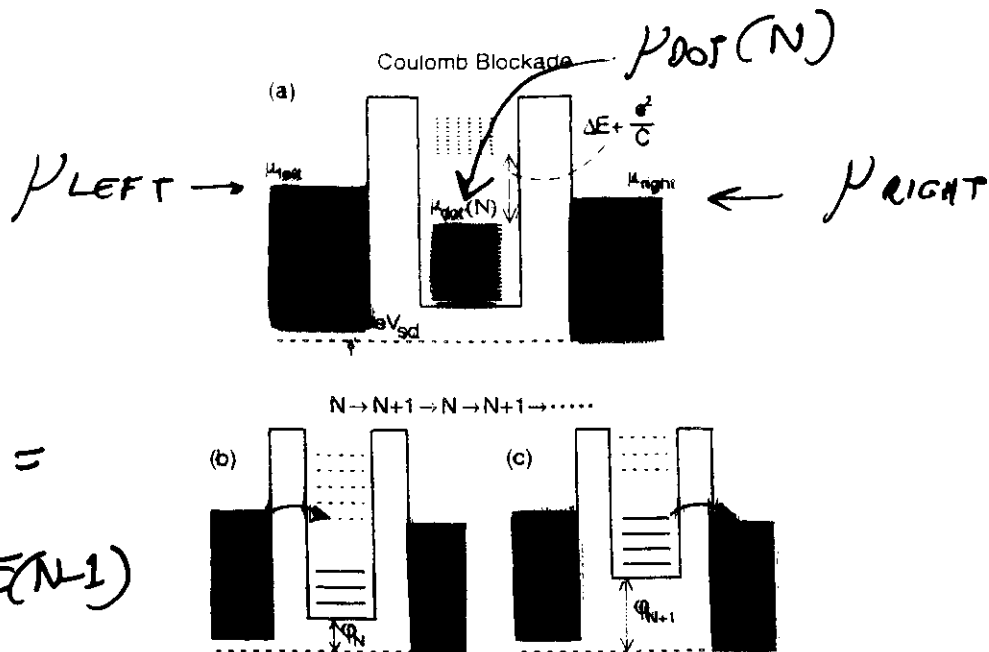


Figure 2.1. Potential landscape through a quantum dot. The states in the 2D reservoirs are filled up to the electrochemical potentials μ_{left} and μ_{right} which are related via the external voltage $V_{sd} = (\mu_{left} - \mu_{right})/e$. The discrete 0D-states in the dot are filled with N electrons up to $\mu_{dot}(N)$. The addition of one electron to the dot would raise $\mu_{dot}(N)$ (i.e. the highest solid line) to $\mu_{dot}(N+1)$ (i.e. the lowest dashed line). In (a) this addition is blocked at low temperature. In (b) and (c) the addition is allowed since here $\mu_{dot}(N+1)$ is aligned with the reservoir potentials μ_{left}, μ_{right} by means of the gate voltage. (b) and (c) show two parts of the sequential tunneling process at the same gate voltage. (b) shows the situation with N and (c) with $N+1$ electrons on the dot.

(FROM KOUWENOVICH et al., TO BE PUBLISHED)

WE IMPOSE $\mu_{LEFT} \approx \mu_{RIGHT} = \mu_{ext}$ ($V_{SD} \approx 0$).

VARYING V_{gate} , WHEN

$$\boxed{\mu_{dot} = \mu_{ext}} \Rightarrow$$

CONDUCTANCE PEAK
(Coulomb oscillation)

- OUR GOAL IS TO PREDICT COULOMB OSCILLATIONS
- NAMELY, WE TRY TO CALCULATE

$$\mu_{\text{dot}}(N) = E(N) - E(N-1)$$

$E(N)$ IS THE N -ELECTRON GROUND STATE ENERGY IN THE QD

- WE ALSO INTRODUCE AN EXTERNAL MAGNETIC FIELD $\vec{B} = B \hat{z}$ (IT DOES NOT ALTER CIRCULAR SYMMETRY)

- ADDITION ENERGY SPECTRUM IS GIVEN CONSIDERING

$$\Delta \mu_{\text{dot}}(N) = \mu_{\text{dot}}(N+1) - \mu_{\text{dot}}(N)$$

I.E. THE VARIATION IN THE POTENTIAL ENERGY OF QD REQUIRED TO ADD ANOTHER ELECTRON TO QD.

- SIMPLE THEORIES TO COMPUTE μ_{dot} ARE NOT SATISFACTORY

$\mu(N)$ ↑

(FROM TARUCHA
et al., IBIDEM)

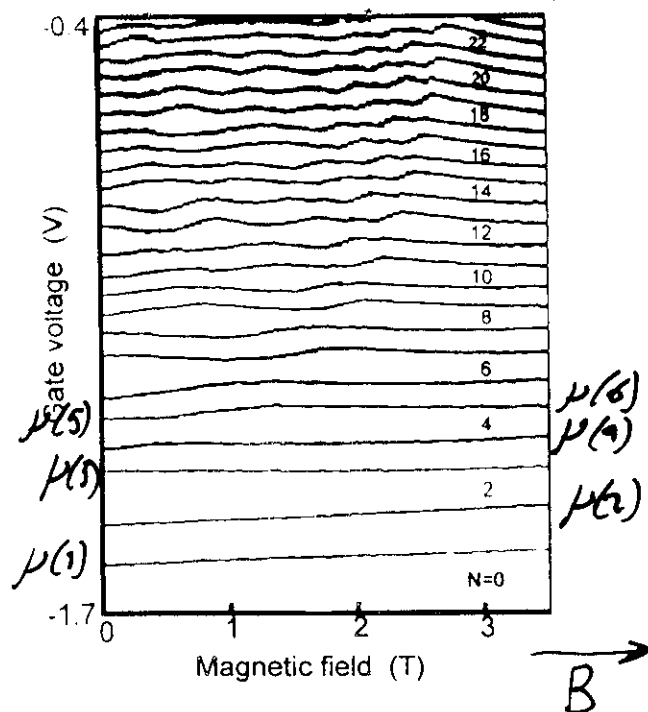


Figure 5.6. Plot of the gate voltage positions of the current peaks in Fig 5.2 vs. magnetic field. (From Tarucha *et al.* [131].)

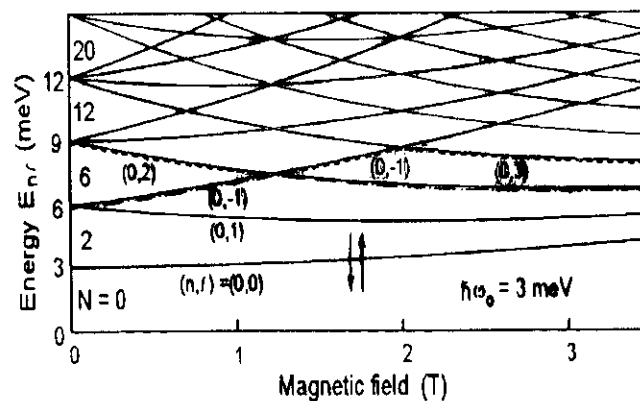


Figure 5.7. Calculated single-particle energy vs. magnetic field for a parabolic potential with $\hbar\omega_0 = 3$ meV. Each state is two fold spin degenerate. The dashed and dot-dashed lines are discussed in the text. (From Tarucha *et al.* [131].)

THINKING OF ELECTRONS AS NON
INTERACTING EXPLAINS VERY
QUALITATIVELY "PAIRING" AND
"WIGGLES" OF μ -CURVES

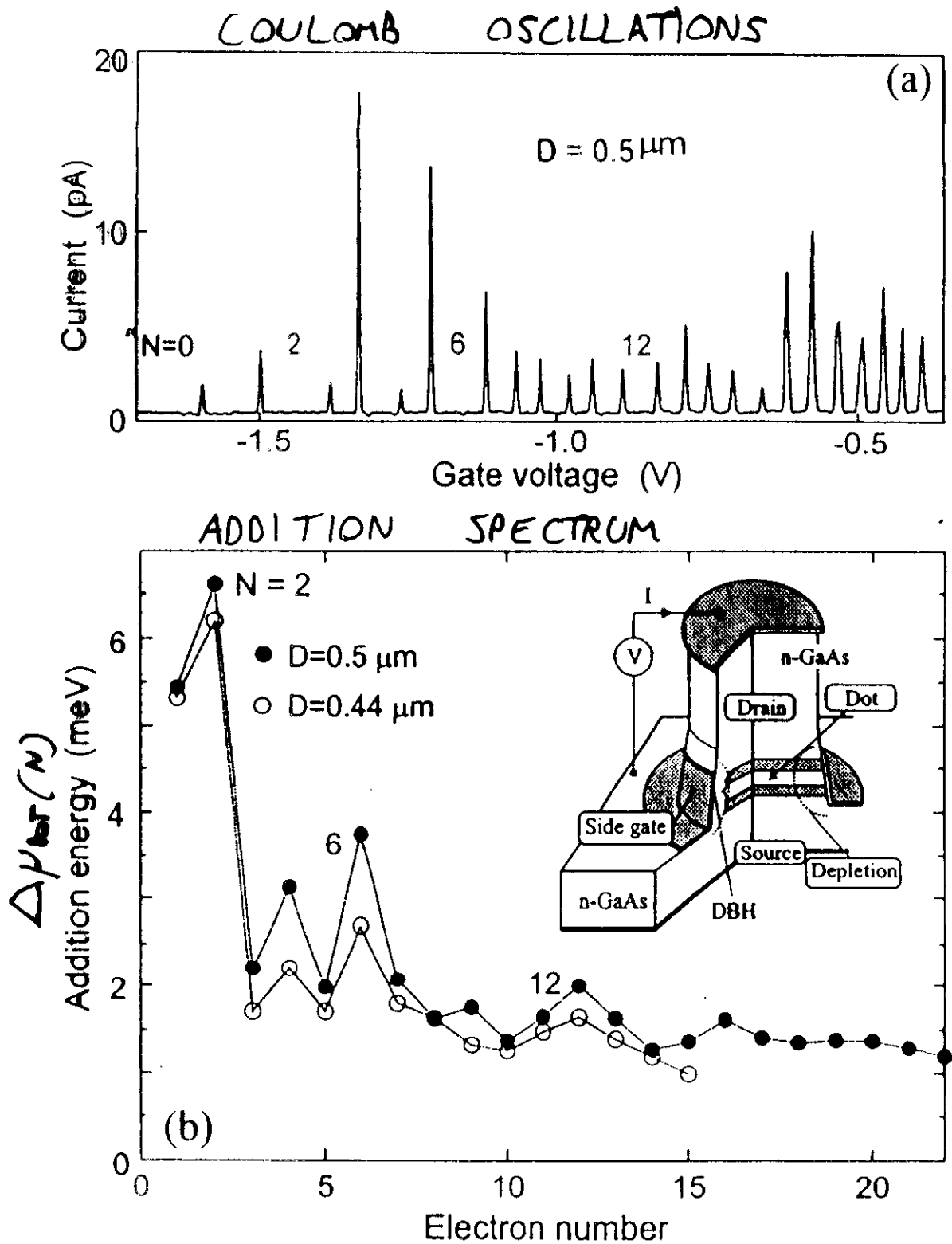
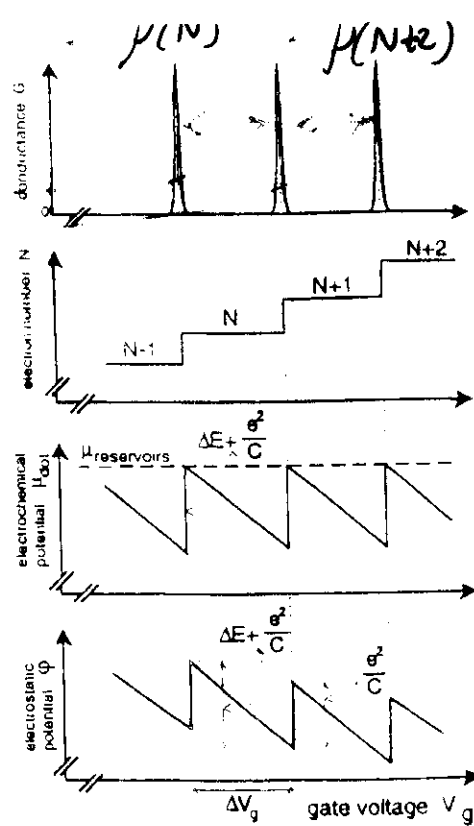


FIG. 1. (a) Coulomb oscillations in the current vs gate voltage at $B = 0$ T observed for a $D = 0.5 \mu\text{m}$ dot. (b) Addition energy vs electron number for two different dots with $D = 0.5$ and $0.44 \mu\text{m}$. The inset shows a schematic diagram of the device. The dot is located between the two heterostructure barriers.

OSCILLATIONS
ARE EQUIDISTANT
IN THIS MODEL



FROM
KOUWENHOVEN
et al., 1990

Figure 2.3. Schematic comparison, as a function of gate voltage, between (a) the Coulomb oscillations in the conductance G , (b) the number of electrons in the dot ($N+i$), (c) the electrochemical potential in the dot $\mu_{dot}(N+i)$, and (d) the electrostatic potential ϕ .

COSTANT CAPACITANCE MODEL
PREDICTS

$$\Delta \mu_{dot}(N) = E(N+1) - E(N) + \frac{e^2}{C}$$

$C \equiv$ COSTANT CAPACITANCE OF QD



PEAKS IN ADDITION SPECTRUM ONLY
AT COMPLETE FILLING OF A SHELL
OF DEGENERATE 2D HARMONIC
OSCILLATOR LEVELS

HOW CAN WE QUANTITATIVELY
EXPLAIN

- PEAKS AT HALF-FILLING IN ADDITION SPECTRUM
- NON EQUIDISTANT COULOMB OSCILLATIONS
- COMPLEX BEHAVIOUR WITH \vec{B} ?

NO SUCH EFFORT UNTIL NOW.



IN SCIENTIFIC LITERATURE WE HAVE

1) EXACT CALCULATIONS

— SEVERE LIMITATIONS ON N (NUMBER OF ELECTRONS)

2) SELF CONSISTENT 2D

HARTREE-FOCK LIKE CALCULATIONS

— PROBLEMS IN DESCRIPTION OF
CORRELATED STATES
(WITH LOW TOTAL SPIN)

Comparison of a Hartree, a Hartree-Fock, and an exact treatment of quantum-dot helium

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We compare energies, pair correlation functions, and particle densities of the ground state of quantum-dot helium in a magnetic field obtained by a Hartree, a Hartree-Fock (HF), and an exact treatment. The exact and HF results for the triplet state agree well, which illustrates the importance of the exchange interaction for systems of few electrons. The results for the singlet state differ significantly and we show that this is caused by a lack of correlation between the angular momenta of the electrons in the HF approximation.

Figure 3 shows the energies E_Θ for the states $|\Theta\rangle = |000\rangle$ and $|\Theta\rangle = |011\rangle$ as a function of the magnetic field achieved by exact diagonalization, Hartree, and HF calculations. While for the $M = 1$ ground state the energies of the HF and exact calculations nearly coincide within the numerical accuracy [HF: (13.36 ± 0.05) meV; exact: (13.26 ± 0.02) meV], they differ for the $M = 0$ ground state. The difference is usually denoted as correlation energy.

The correlations, neglected in the HF calculation, become transparent in a comparison of the ground-state wave functions calculated by the different methods. Table I lists the most important coefficients $d_{\Theta;ab}$ [Eq. (7)]

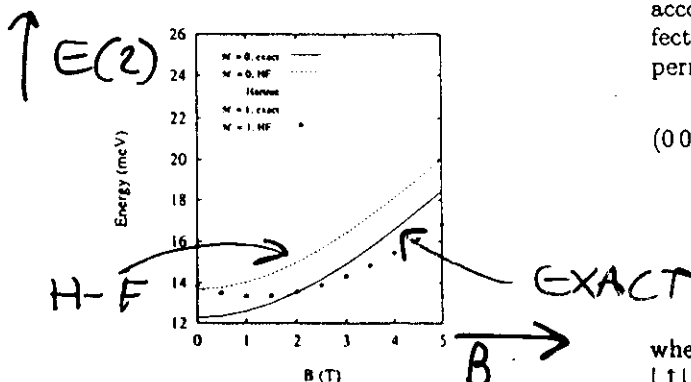


FIG. 3. Ground-state energies from Hartree, HF, and exact calculations as a function of the magnetic field. (Confining energy $\hbar\Omega = 3.37$ meV, material constants for GaAs.)

In contrast, the expansion of the exact wave function allows for all combinations of M_1 and M_2 with fixed sum M .

For the $M = 0$ state the importance of combinations $M_1 = M$, $M_2 = -M$ ($M > 0$) increases with increasing strength of the Coulomb interaction relative to the effective confining energy $\hbar\Omega_{\text{eff}}$. Because of their larger spatial extent, wave functions with larger angular momenta tend to decrease the interaction energy. To demonstrate this, we estimate the interaction contribution to the total energy for the different $|000\rangle$ states, only taking into account the states listed in Table I. Including the effect of the symmetry of the singlet state under particle permutation the interaction energy is given by

$$\begin{aligned} \langle 00|V|00\rangle = & 2 \frac{\sqrt{\pi} e^2}{2\kappa\lambda} \{ d_{00,00,00}^2 + (d_{00,10,00} - d_{00,0-1,01})^2 \\ & + \frac{3}{4} (d_{00,10,00} + d_{00,0-1,01})^2 \\ & + d_{00,00,00} (d_{00,10,00} + d_{00,0-1,01}) \}, \end{aligned} \quad (17)$$

where the factor 2 accounts for the two spin functions $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ which are not coupled by the Coulomb interaction. (Throughout the following paragraph the spin quantum number is omitted; the matrix element was calculated by transforming to CM and relative coordinates.)

Numerical simulation of shell-filling effects in circular quantum dots

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(Received 15 November 1996)

We have computed the capacitive energy associated with the addition of each electron to a circular quantum dot, reproducing the shell-filling behavior as reported in previous simulations and recently found experimentally. We derived quantitative estimates for the shape of the confining potential and for the dot radius in the experiments. Our results show that the succession of shell-filling events differs for the case of a realistic self-consistent potential from that predicted by a single-electron approximation and with an idealized parabolic potential. [S0163-1829(97)51808-X]

Recent measurements by Tarucha *et al.*,¹ using vertical quantum dots, have provided experimental evidence of the shell structure of addition energies as predicted in Refs. 2–4. This has been possible through a sophisticated technology^{5,6} that has allowed the fabrication of smaller and geometrically more controllable quantum dots. The vertical confinement

where \hbar is the reduced Planck constant, m^* the effective mass of the electron, ρ the radial coordinate, and ϕ the angular coordinate. The material parameters for $\text{In}_{0.05}\text{Ga}_{0.95}\text{As}$ have been computed with a linear interpolation between the parameters of InAs and GaAs, which gives $m^* = 0.0648m_0$ and $\epsilon_r = 12.98$. The total potential $V(\rho)$

RAPID COMMUNICATIONS

R4880

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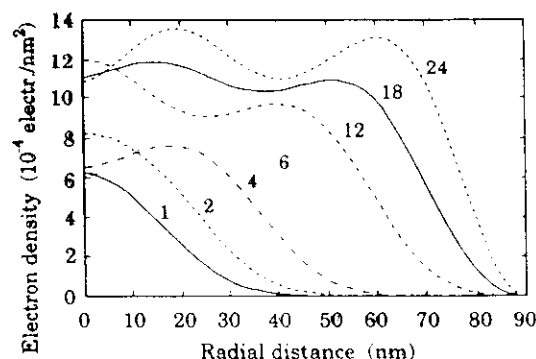


FIG. 1. Electron density as a function of dot radius, for different electron numbers: the geometric dot radius is 90 nm and the confinement potential is parabolic, with $\hbar\omega = 3$ meV.

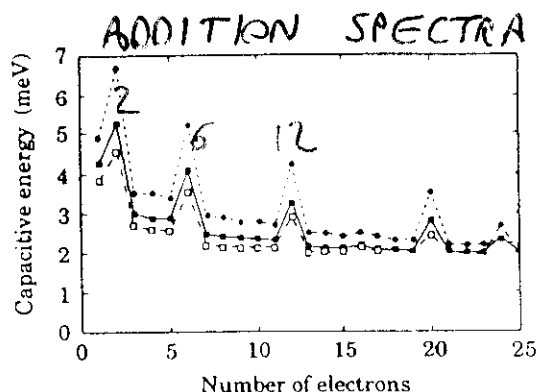


FIG. 2. Self-consistent capacitive energy of a quantum dot with a radius of 90 nm as a function of the number of electrons, including a parabolic confinement potential defined by $\hbar\omega = 4$ (solid dots), 3 meV (solid squares), and 2.5 meV (empty squares).

tion. This is the consequence of the fact that the interaction energy scales with $1/R_e$, R_e being the effective radius over which the electron wave function is spread, while the confinement energy scales with $1/R_e^2$.⁹ Thus, for increasing dot size, the Coulomb energy becomes more and more important, leading to a very stiff self-consistent problem.

2 are for dots with the same geometrical radius, but with a confinement potential with $\hbar\omega = 4$ (solid dots) 2.5 meV (empty squares).

Examining the detailed features of these results, we notice that peaks occur in more positions than those predicted on

WE INTRODUCE THE MANY BODY PROTOTYPE HAMILTONIAN FOR CORRELATED ELECTRONIC STATES (FOR A LATTICE OF QDS)

$$\hat{H} = \sum_{\alpha} \epsilon_{\alpha} \sum_{i, \sigma} \hat{n}_{i\sigma} + \sum_{\alpha, \beta} \sum_{\langle i, j \rangle} t_{i\alpha, j\beta} \times \\ \times \sum_{\sigma} \hat{c}_{i\alpha\sigma}^{\dagger} \hat{c}_{j\beta\sigma} + U_{\alpha\beta} \sum_i \hat{n}_{i\alpha\uparrow} \hat{n}_{i\beta\downarrow} + \\ + \frac{1}{2} \sum_{\alpha, \beta} (U_{\alpha\beta} - J_{\alpha\beta}) \sum_{i, \sigma} \hat{n}_{i\alpha\sigma} \hat{n}_{i\beta\sigma}$$

$\hat{c}_{i\alpha\sigma}^{\dagger} \equiv$ CREATION OPERATOR FOR AN ELECTRON WITH ENERGY ϵ_{α} AND SPIN σ ON THE i -TH QD. ($\hat{n}_{i\alpha\sigma} = \hat{c}_{i\alpha\sigma}^{\dagger} \hat{c}_{i\alpha\sigma}$)

$t_{i\alpha, j\beta} \equiv$ "HOPPING" COEFFICIENT BETWEEN i -TH AND j -TH QDS.

$U_{\alpha\beta}, J_{\alpha\beta} \equiv$ COULOMB AND EXCHANGE INTEGRALS BETWEEN α AND β LEVELS.

$\alpha \equiv$ SET OF QUANTUM NUMBERS. FOR THE 2D HARMONIC OSCILLATOR, $\alpha = (n, m)$.

THIS IS THE GENERALIZED HUBBARD MODEL.

IN THE CASE OF A SINGLE QD, H IS:

$$\begin{aligned} \hat{H} = & \sum_{\alpha, \sigma} \epsilon_{\alpha} \hat{n}_{\alpha \sigma} + \\ & + \sum_{\alpha, \beta} U_{\alpha \beta} \hat{n}_{\alpha \uparrow} \hat{n}_{\beta \downarrow} + \quad \leftarrow \text{IT COUPLES ANTI-PAALLEL SPINS} \\ & + \frac{1}{2} \sum_{\alpha, \beta} \sum_{\sigma} (U_{\alpha \beta} - J_{\alpha \beta}) \hat{n}_{\alpha \sigma} \hat{n}_{\beta \sigma} \quad \leftarrow \text{IT COUPLES PARALLEL SPINS} \end{aligned}$$

WITH

$$U_{\alpha \beta} = e^2 \int d\vec{r} \int d\vec{r}' \frac{|\phi_{\alpha}(\vec{r})|^2 |\phi_{\beta}(\vec{r}')|^2}{K |\vec{r} - \vec{r}'|}$$

$$J_{\alpha \beta} = e^2 \int d\vec{r} \int d\vec{r}' \frac{\phi_{\alpha}^*(\vec{r}) \phi_{\beta}^*(\vec{r}') \phi_{\alpha}(\vec{r}') \phi_{\beta}(\vec{r})}{K |\vec{r} - \vec{r}'|}$$

$\phi_{\alpha}(\vec{r}) \equiv$ REAL SPACE EIGENFUNCTION.

THE ENERGY $E(N)$ OF A STATE WITH N ELECT. IS

$$\begin{aligned} E(N) = & \sum_{\alpha \sigma} \epsilon_{\alpha} \langle \hat{n}_{\alpha \sigma} \rangle + \frac{1}{2} \sum_{\alpha \beta \sigma} \left[U_{\alpha \beta} \langle \hat{n}_{\beta - \sigma} \rangle \right. \\ & \left. + (U_{\alpha \beta} - J_{\alpha \beta}) \langle \hat{n}_{\beta \sigma} \rangle \right] \langle \hat{n}_{\alpha \sigma} \rangle \end{aligned}$$

(*)

NOTE THAT H IS A MANY BODY HAMILTONIAN, BUT IT IS EXACTLY SOLVABLE, BECAUSE

$$[\hat{H}, \hat{n}_{\alpha r}] = 0$$

SO MANY BODY EIGENFUNCTIONS ARE SIMPLE SLATER DETERMINANTS OF SINGLE PARTICLE EIGENFUNCTIONS AND, FIXED N AND TOTAL SPIN S , WE DERIVE $E(N)$ FROM (*) JUST LOOKING FOR THE MINIMUM CONFIGURATION ENERGY. CONTRARY TO USUAL HUBBARD APPROACHES, U AND J ARE CALCULATED (NOT PARAMETERS).

WITHIN THE MODEL,
THERE IS NO APPROXIMATION

- THE METHOD IS CONCEPTUALLY SIMPLE, AND THE CALCULATION STRAIGHTFORWARD
- AT THE SAME TIME, IT PERMITS GREAT ACCURACY TO MIMIC EXPERIMENTAL SYSTEM
- IT HAS GREAT POTENTIALITIES :
 - EXACT EXCITED STATES
 - EXTENSION TO SYSTEMS OF COUPLED QDs



- EQUATION (*) FOR $E(N)$ IS FORMALLY EQUIVALENT TO HARTREE-FOCK ENERGY
- WE FOUND THAT THE METHOD DOESN'T ACCOUNT FOR EXPERIMENTAL RESULTS IN THE LIMIT OF VERY LOW ENERGY SPLITTINGS $\hbar\omega_0$ BETWEEN DIFFERENT SHELLS

CALCULATION INGREDIENTS

WE MIMICKED EXPERIMENT OF TARUCHA et al. (1990)

$$V(r, y) = \frac{1}{2} m^* \omega_0^2 r^2 \quad (\text{AT } B=0)$$

$$V(z) = \begin{cases} V_0 & \text{IF } z > \frac{L}{2} \\ 0 & \text{IF } \frac{L}{2} > z > -\frac{L}{2} \\ V_0 & \text{IF } z < -\frac{L}{2} \end{cases}$$

$$\frac{m^*}{m_0} = \begin{cases} 0.65 & \text{IN THE DOT} \\ 0.80 & \text{IN THE BARRIERS} \end{cases}$$

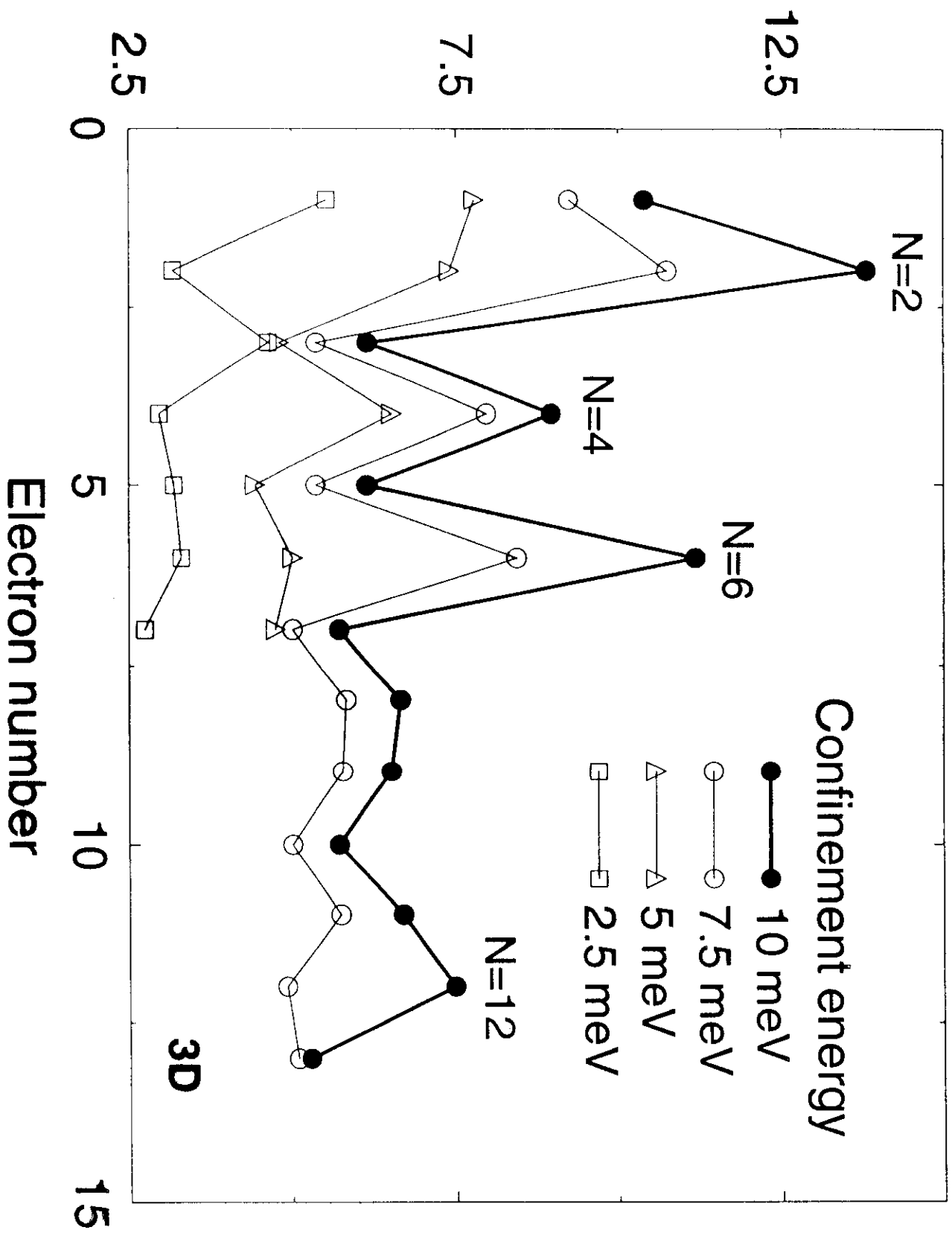
$$\chi = 12.98 \quad (\text{In}_{0.05}\text{Ge}_{0.95}\text{As}) \quad L = 120 \text{ \AA}$$

$$V_0 = 200 \text{ meV}$$

WE USED 4 DIFFERENT VALUES OF $\hbar\omega_0$
(CORRESPONDING TO DIFFERENT DIAMETERS OF
THE DOT)

$$\hbar\omega_0 = 2.5, 5, 7.5, 10 \text{ meV}$$

Capacitive energy (meV)



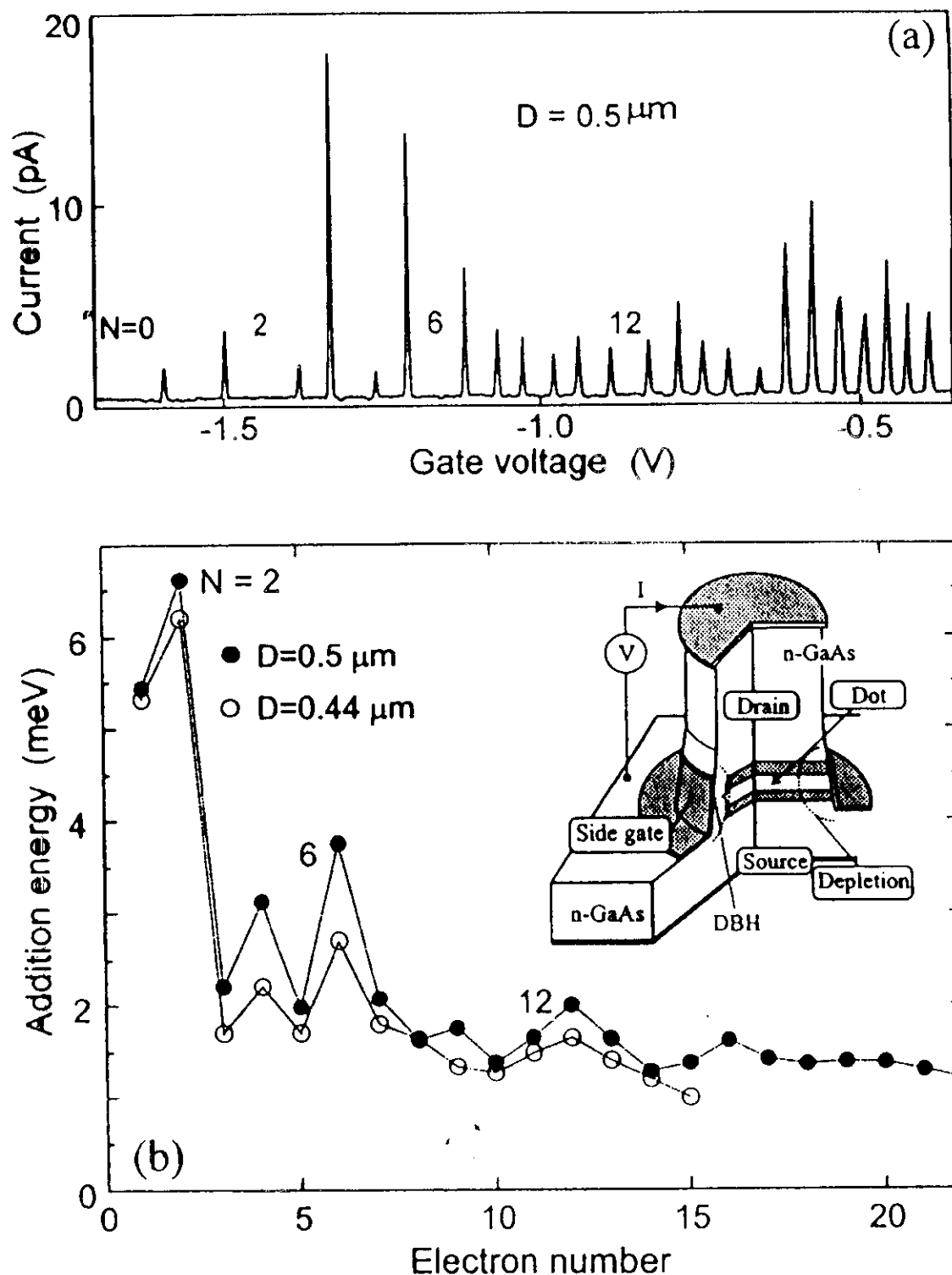


FIG. 1. (a) Coulomb oscillations in the current vs gate voltage at $B = 0$ T observed for a $D = 0.5 \mu\text{m}$ dot. (b) Addition energy vs electron number for two different dots with $D = 0.5$ and $0.44 \mu\text{m}$. The inset shows a schematic diagram of the device. The dot is located between the two heterostructure barriers.

WE FOUND, IN THE ADDITION SPECTRA, PEAKS AT THE FILLING ($N=2, 6, 12$) AND HALF-FILLING ($N=4, 9$) OF SHELLS, AT $B=0$.

THESE SHELLS ARE THOSE OF 2D HARMONIC OSCILLATOR LEVELS (SEE FIGURE).

ELECTRON-ELECTRON INTERACTION PLAYS A FUNDAMENTAL ROLE IN EXPLAINING SUCH FILLINGS: IT IS RESPONSIBLE FOR HUND'S RULE IN FILLING LEVELS.

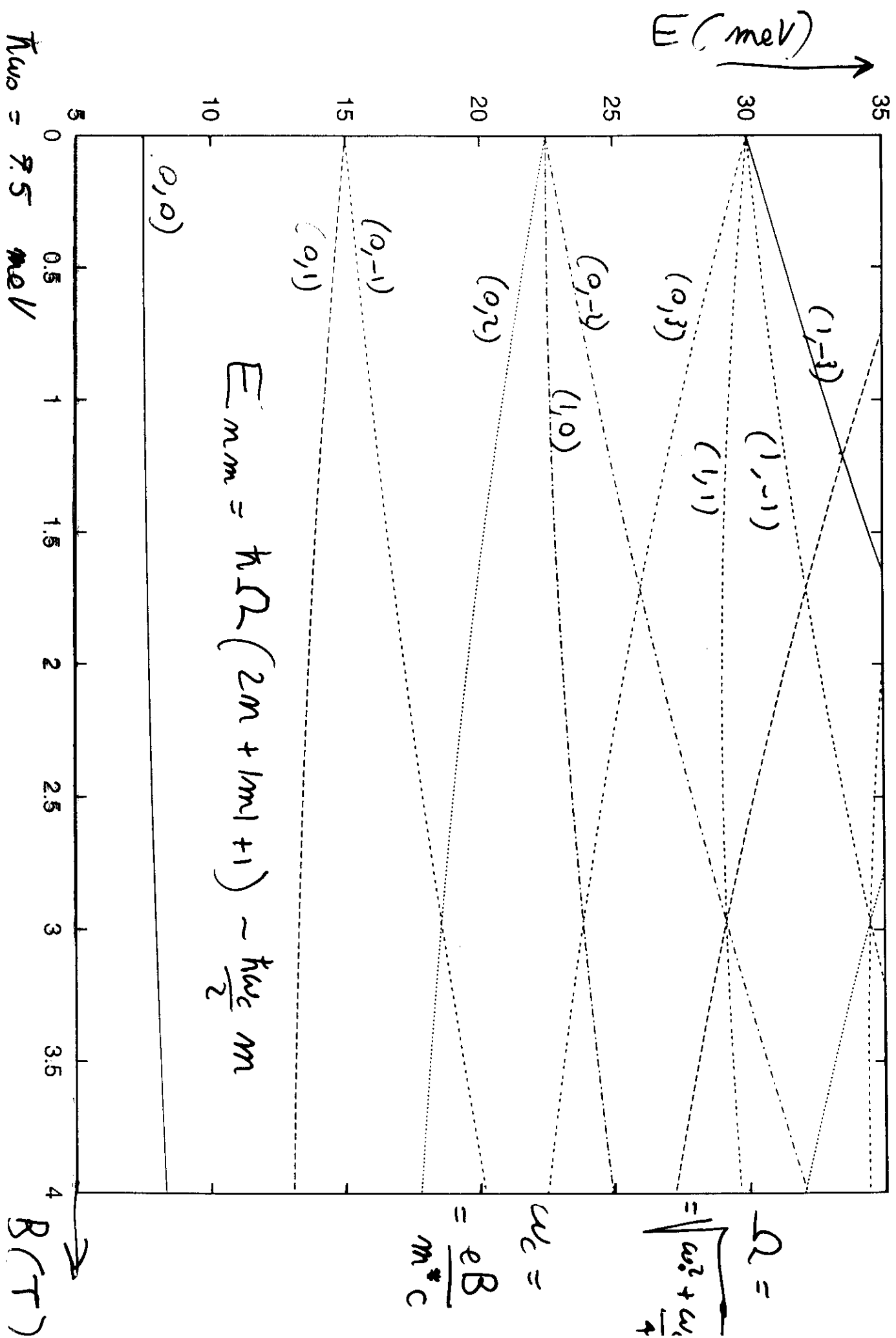
IN FACT, WE FOUND A FILLING RULE (AS IN ATOMIC PHYSICS) TO FILL LEVELS OF QD (~~NEVER THEORETICALLY REPORTED~~):

- 1) ELECTRONS CONFIGURE TO COMPLETELY FILL THE OUTER SHELL THEMSELVES
- 2) WITHIN A SHELL, THEY ARE PLACED IN SUCH A WAY TO MAXIMIZE TOTAL SPIN S (I.E., WITH PARALLEL SPINS AS MUCH AS POSSIBLE)
- 3) COMPATIBLY WITH S , THEY MAXIMIZE

$$\sum_i |L_{z_i}| \quad (L_{z_i} = -\hbar m)$$

(NOTE THAT, DESPITE REAL ATOMS, L_z AND NOT \vec{L} IS CONSERVED, $m = 0, \pm 1, \pm 2, \dots$)

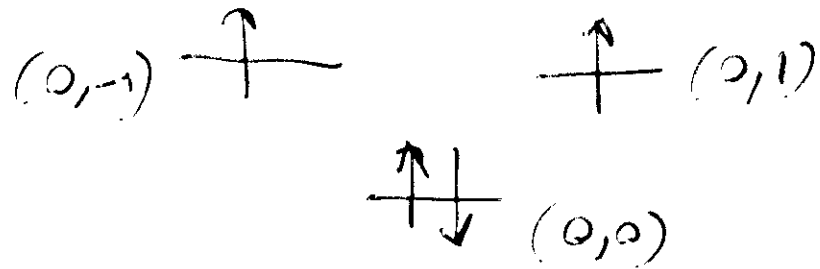
SINGLE PARTICLE 2D HARMONIC OSCILLATOR ENERGY LEVELS



THIS EXPLAINS PEAKS AT HALF FILLING:

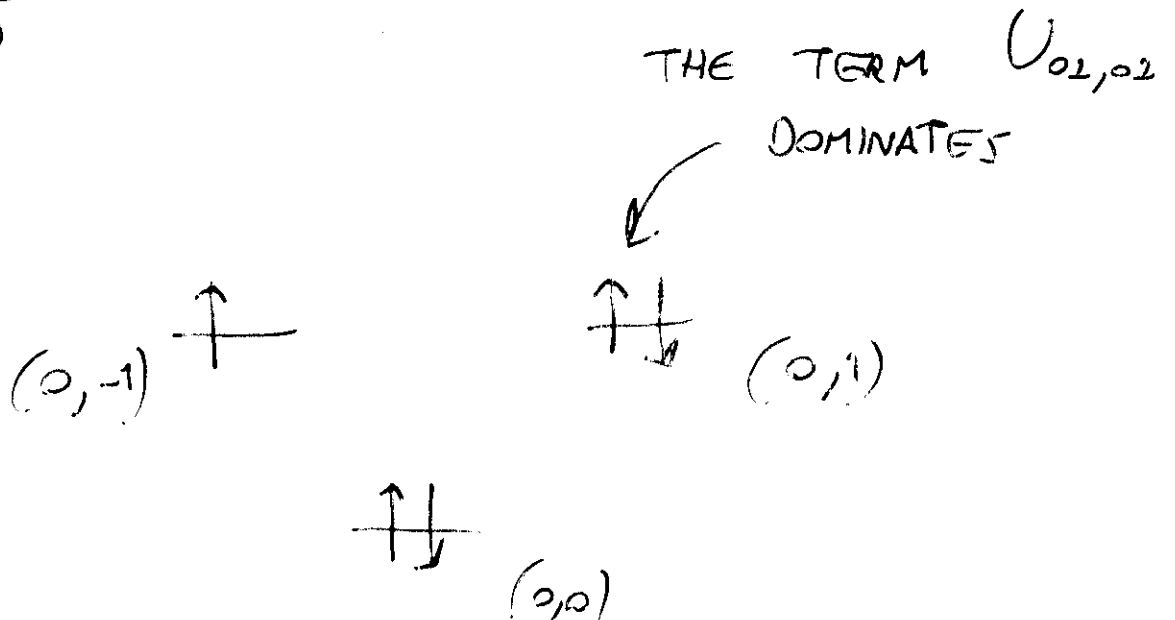
ELECTRONS CONFIGURE IN SUCH A WAY TO MAXIMIZE SPIN (EXCHANGE INTERACTION), AND WE HAVE THE MAXIMUM VALUE OF TOTAL SPIN AT HALF FILLING ($N=4, 9$)

ex. $N=4$



ADDING AN ELECTRON COSTS, IN ADDITION SPECTRUM, THE COULOMB REPULSION U BETWEEN TWO ELECTRONS ON THE SAME LEVEL

ex. $N=5$



WHAT IS THE ORIGIN OF THESE RULES?
THEY ARE BASED ON A BALANCE
BETWEEN ϵ , U AND $U-J$ TERMS IN \hat{H} ,
TO MINIMIZE GROUND STATE ENERGY.
RULE 1) ASSURES THAT THE SUM OF
ONE PARTICLE ENERGIES ϵ HAS A MINIMUM
VALUE.

RULE 2) CAUSES THE SUM OF COULOMB
INTEGRALS $U_{\alpha\alpha}$ REFERRED TO THE SAME
LEVEL TO BE MINIMIZED. THESE $U_{\alpha\alpha}$
TERMS ARE THE DOMINANT MANY BODY TERMS

RULE 3) ASSURES THAT U AND J INTEGRALS
ARE MINIMIZED : IN FACT, IF m IS
RAISED, $|\phi_{nm}(\vec{r})|^2$ SPLITS IN SPACE,
AND $U_{nm;x}$ AND $J_{nm;x}$ ARE LOWERED.

IN THE SAME WAY, HUND'S RULE
EXPLAINS "WIGGLES" IN THE μ - B PLOT.

B ENERGETICALLY FAVOURS CONFIGURATIONS
WITH MAXIMUM $m_{\text{TOT}} = \sum_i m_i$.

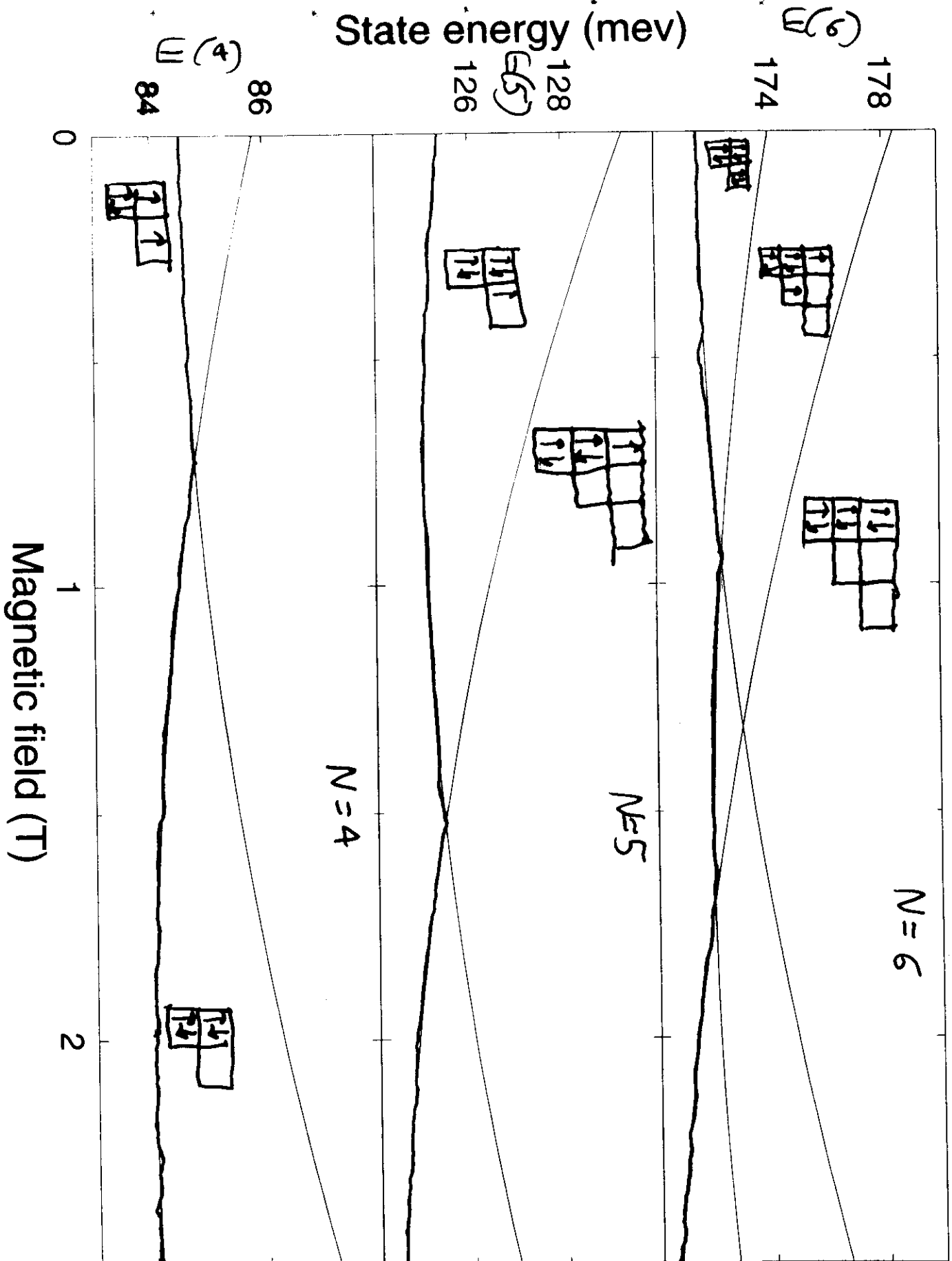
HOWEVER, HUND'S RULE FAVOURS CONFIGURATIONS
WITH S MAXIMUM, SO, TURNING ON B ,

FOR A CERTAIN CRITICAL VALUE THERE
WILL BE A "WIGGLE" IN THE μ - B PLOT

CORRESPONDING TO THE PROMOTION OF
AN ELECTRON FROM A ~~VALUE~~^{LEVEL} WITH
LOWER m TO A LEVEL WITH

HIGHER m (POSSIBLY WITH SPIN FLIP)

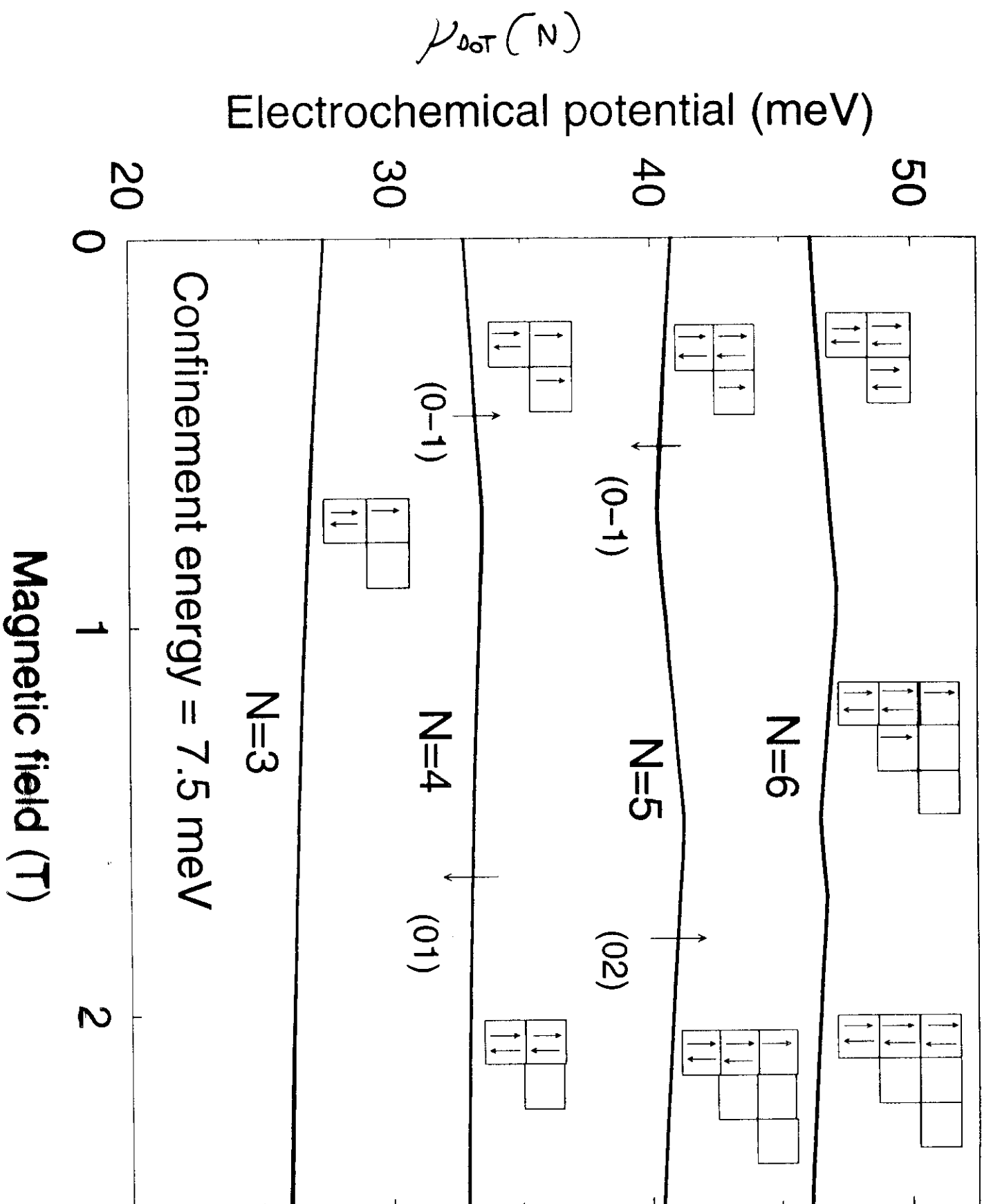
(SEE FIGURE).

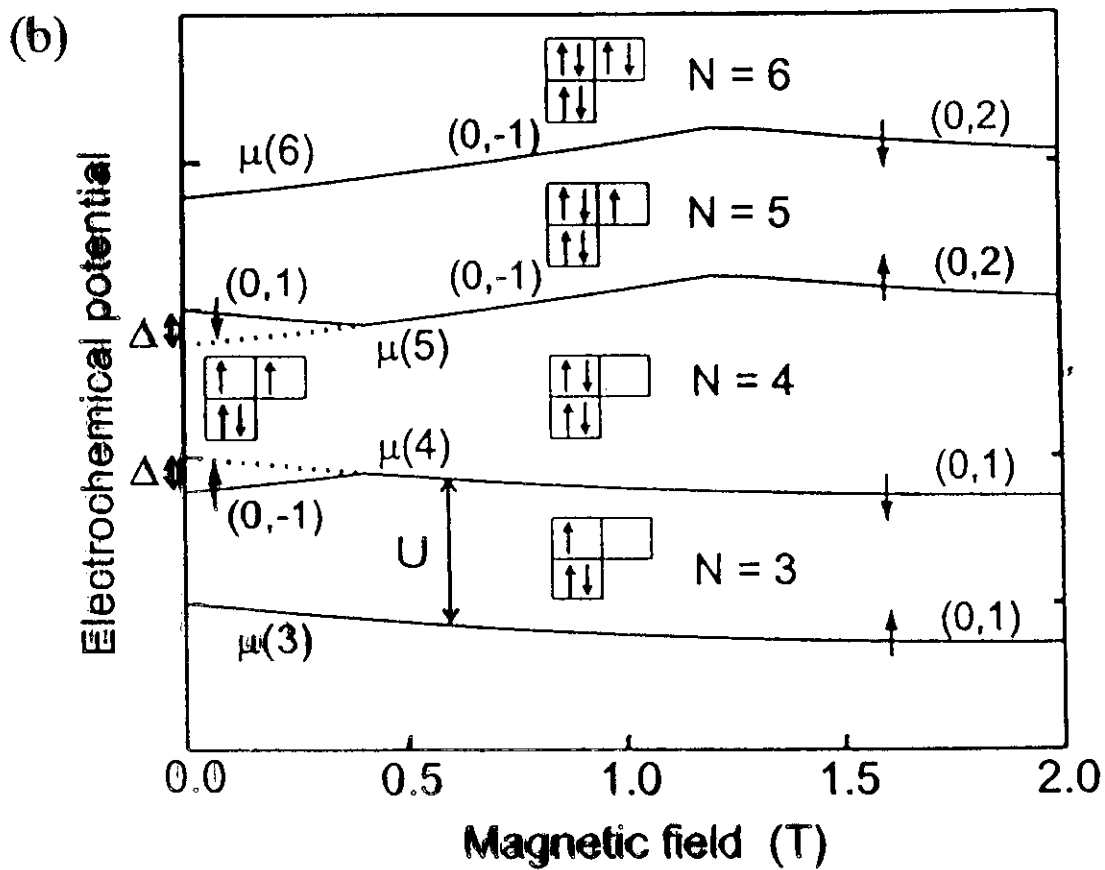
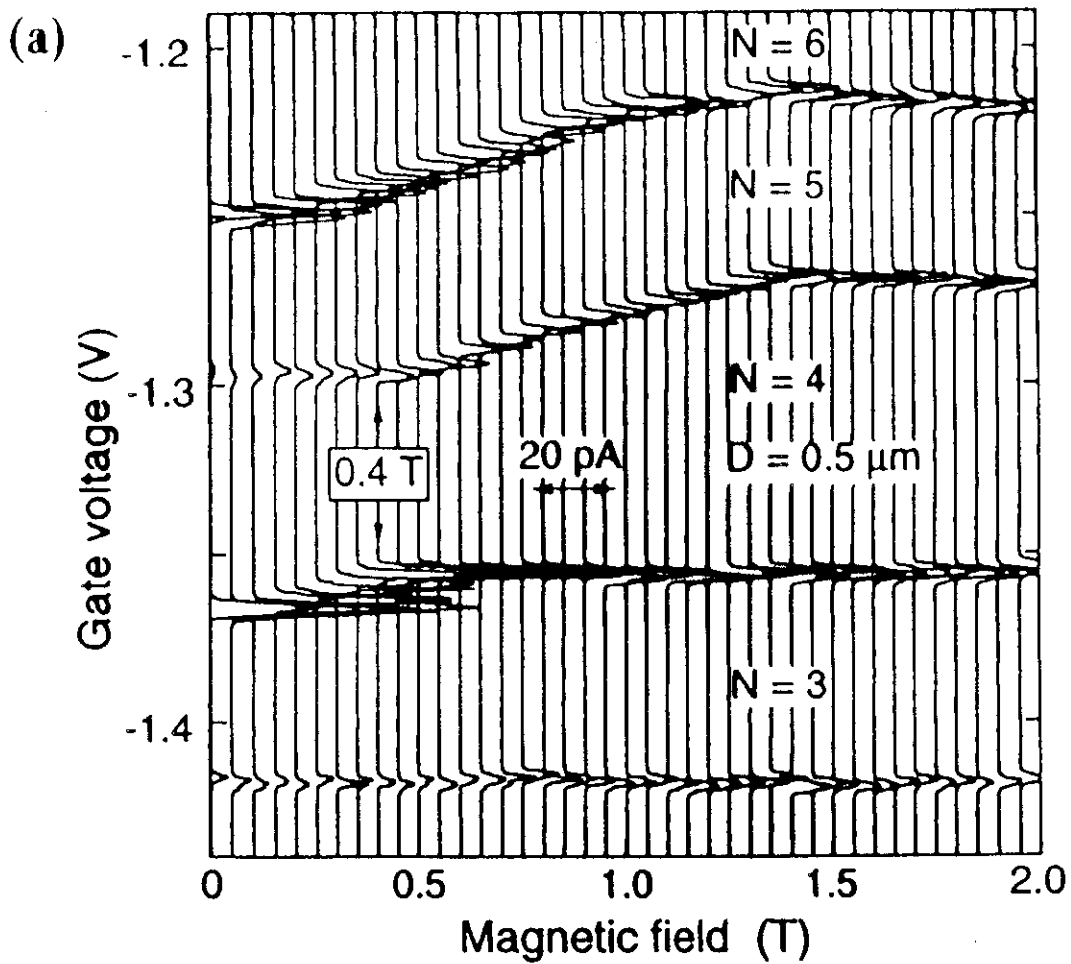


LEGEND

(n, m)

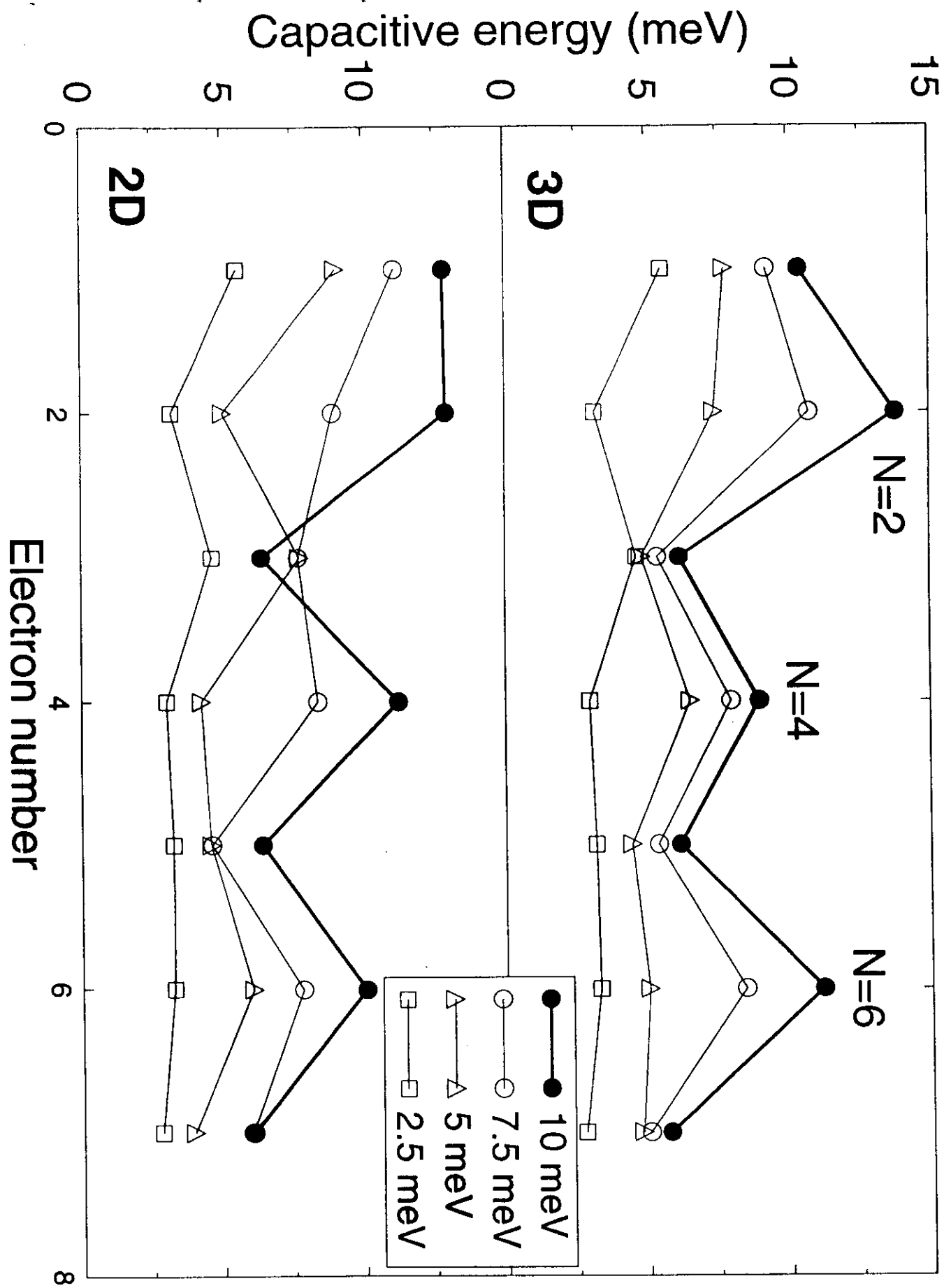
0,2	1,0	0,
0,1	0,-1	
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WE SEPARATELY COMPUTED
ADDITION SPECTRA DESCRIBING ~~QDS~~
THE DOT AS A 2D DISK AND AS
A 3D STRUCTURE, WITH A SPATIAL
EXTENSION ALONG Z AXIS.

IN BOTH CASES WE FOUND THAT THE
METHOD DOESN'T ACCOUNT FOR
EXPERIMENTAL RESULTS IN THE
LIMIT OF LOW CONFINEMENT POTENTIAL
ENERGY $\hbar\omega_0$: HOWEVER, THIS LIMIT
IS MUCH HIGHER IN 2D CASE THEN
IN 3D.

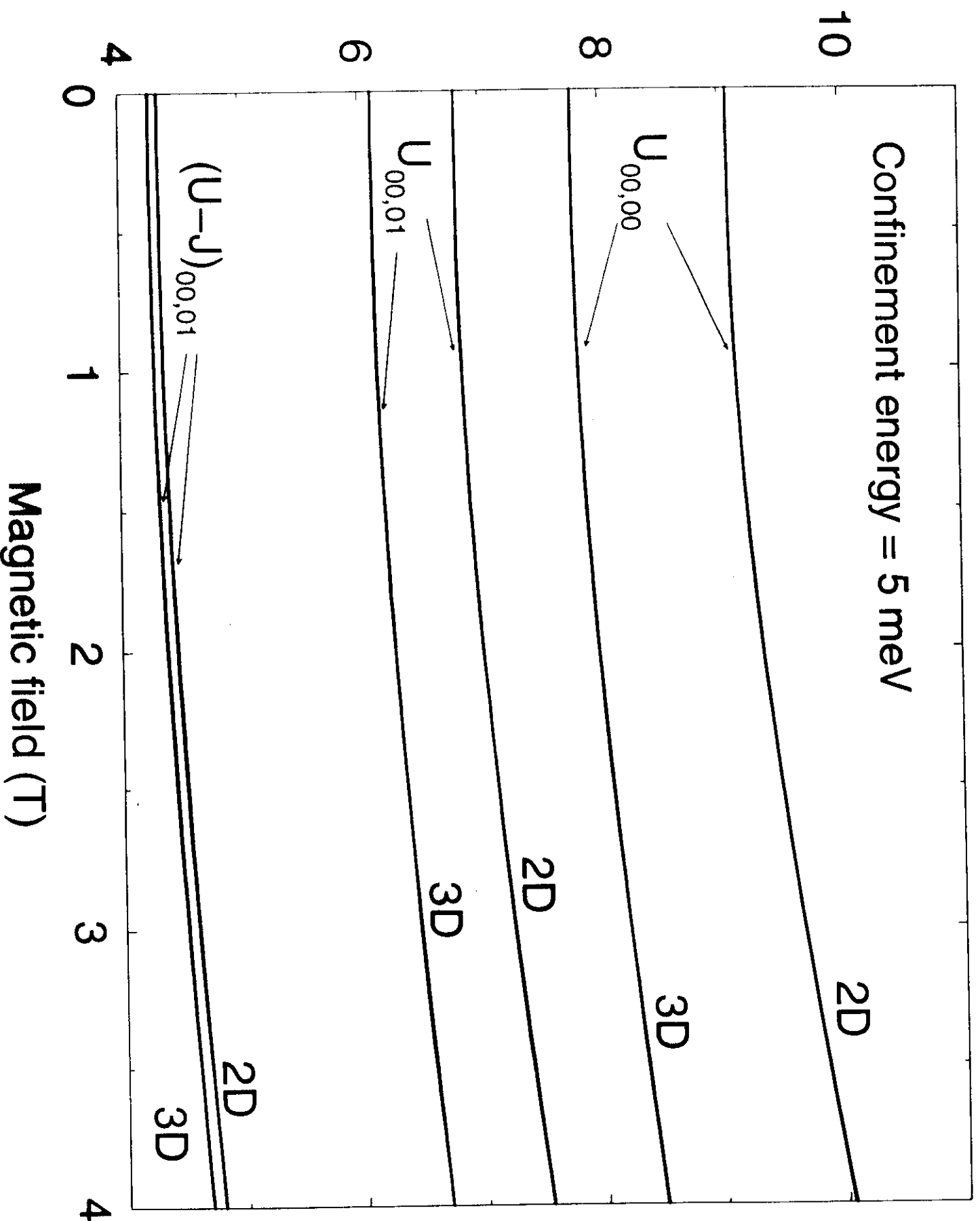


ONLY A 3D COMPUTATION OF U AND J
GUARANTEES THE SHELL FILLING AS WE
STATED IT. (SEE FIGURE)

THE 2D TREATMENT
OVERESTIMATES U TERMS (THAT
REPEL ELECTRONS WITH ANTIPARALLEL SPIN,
WHILE $(U - J)$ TERMS (THAT REPEL
ELECTRON WITH PARALLEL SPIN) DON'T
REALLY CHANGE MUCH:

THIS IMPEDES THE COMPLETE
FILLING OF A SHELL (SEE FIGURE).

U and J integrals (meV)



CONCLUSIONS

- CONCEPTUALLY SIMPLE AND POWERFUL METHOD
- THEORETICAL EVIDENCE FOR HUND'S RULE
- ADDITION SPECTRA IN AGREEMENT WITH EXPERIMENTAL RESULTS
- FUNDAMENTAL ROLE OF 3D DESCRIPTION OF THE DOT

THANKS TO C. CALANDRA FOR USEFUL DISCUSSIONS. WORK IN PART SUPPORTED BY THE EC THROUGH THE TMR-NETWORK "ULTRAFAST".

