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INTERNATIONAL ATOMIC ENERGY AGENCY
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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SMR.998d - 27

Research Workshop on Condensed Matter Physics
30 June - 22 August 1997
MINIWORKSHOP ON
QUANTUM WELLS, DOTS, WIRES
AND SELF-ORGANIZING NANOSTRUCTURES
11 - 22 AUGUST 1997

"Electronic Structure of Few-Particle Quantum Dots"

PART I

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Outline

- Few Electron Quantum Dots:

  Artificial Atoms

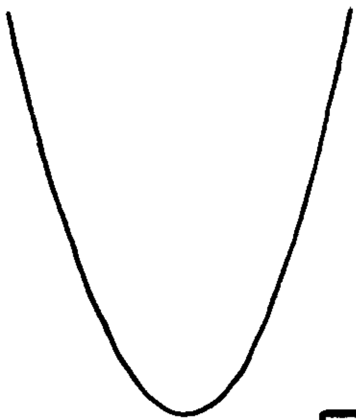
  - QD-Hydrogen: a 2D harmonic oscillator
  - QD-Helium: an illustrative example

- Correlations in Few-Particle Systems

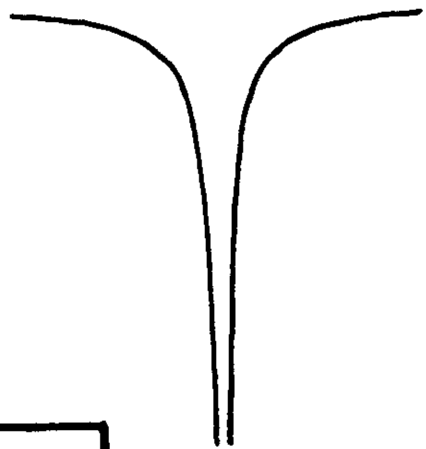
- Chaos induced by Coulomb interaction?

Artificial Atoms

artificial: ~r^2



natural: ~$1/r$



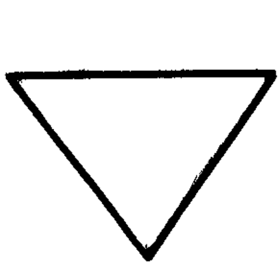
discrete spectrum

number of electrons

↓

"quantum dot element"

Coulomb interaction



kinetic energy

confinement energy

Hamiltonian

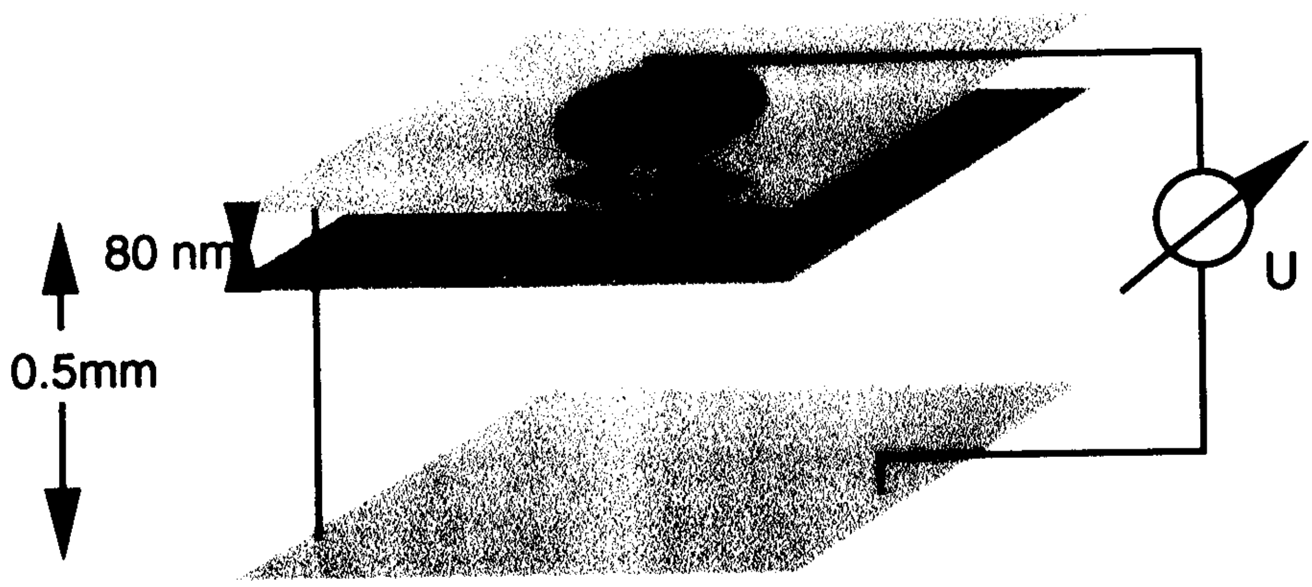
2D-electron in perpendicular magnetic field — Zeeman-energy — Coulomb-interaction

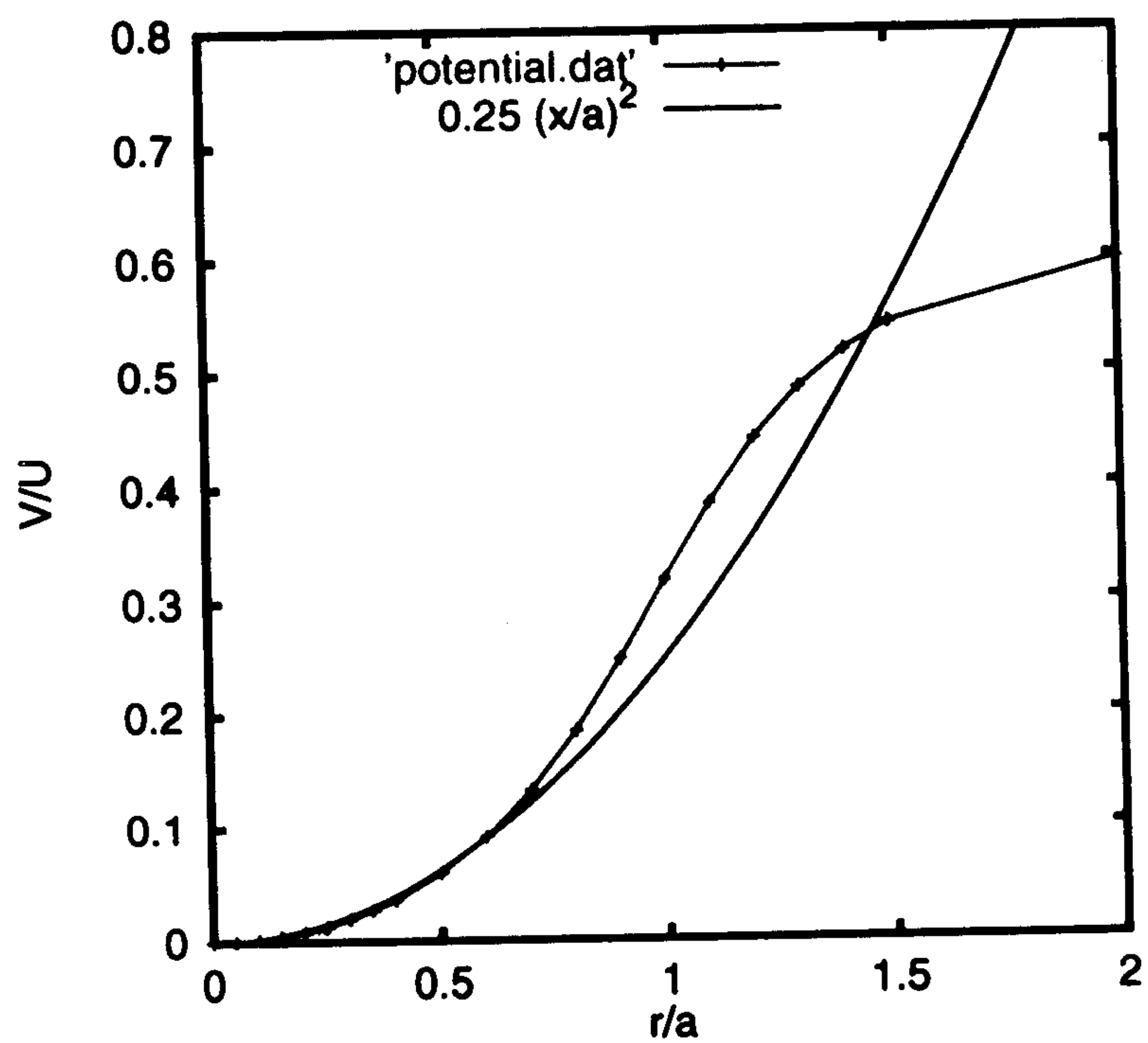
$$\mathcal{H} = \sum_{i=1}^{N_s} \left[\frac{1}{2m^*} \left(\vec{p}_i + \frac{e}{c} \vec{A}(\vec{r}_i) \right)^2 + \frac{g^* \mu_B}{\hbar} \vec{B} \cdot \vec{S}_i + V_{conf}(\vec{r}_i) \right] + \sum_{i<j}^{N_s} \frac{e^2}{\varepsilon |\vec{r}_i - \vec{r}_j|}$$

confining potential

$$V_{conf}(r) = \frac{1}{2} m^* \Omega_0^2 r^2$$

Elektrostatisches Potential





1-Particle Quantum Dot: QD-Hydrogen

$$H_0 = \frac{1}{2m^*}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2 + \frac{1}{2}m^*\Omega_0^2 r^2$$

symmetric gauge

$$= \hbar\Omega_+(a_+^+ a_+ + \frac{1}{2}) + \hbar\Omega_-(a_-^+ a_- + \frac{1}{2})$$

effective confinement frequency

$$\Omega_\pm = \sqrt{\Omega_0^2 + \omega_c^2/4} \qquad \omega_c = \frac{eB}{m^* c}$$

angular momentum

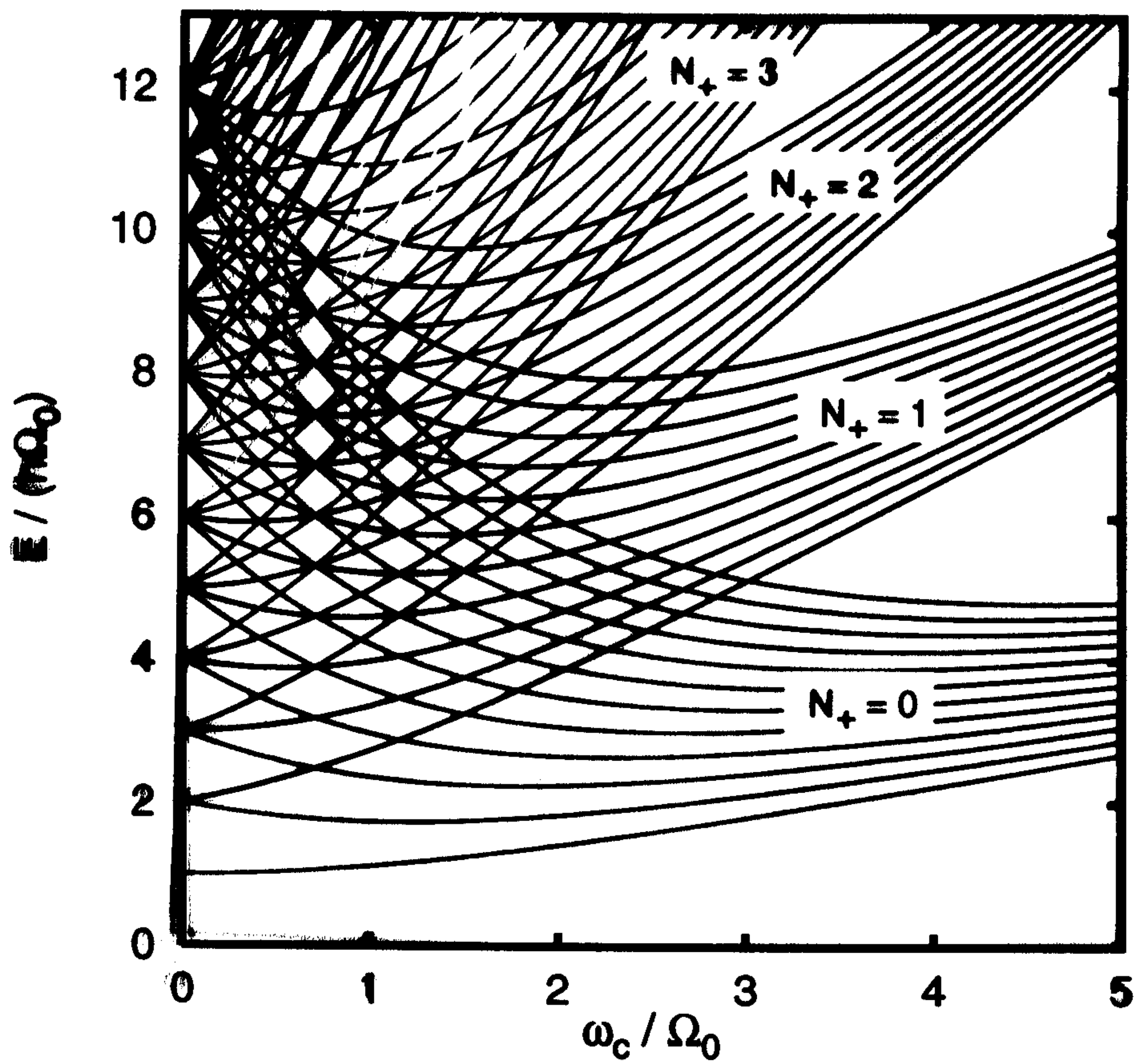
$$L_z = \hbar(a_+^+ a_+ - a_-^+ a_-)$$

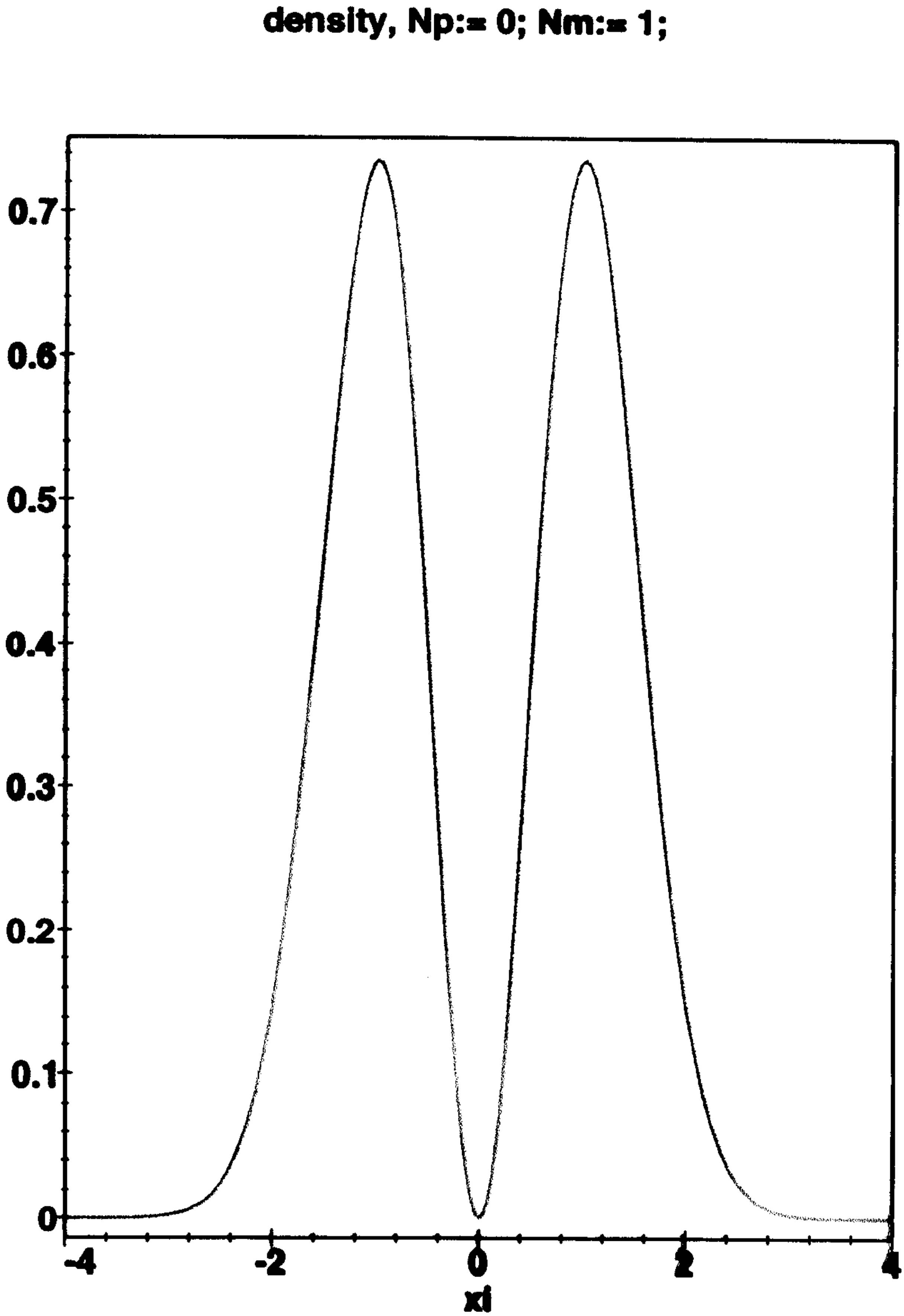
eigenstates $|N_+ N_-\rangle$:
right(+) and left(-) circular polarized modes

s-states: $N_+ - N_- = 0$
p-states: $N_+ - N_- = \pm 1$

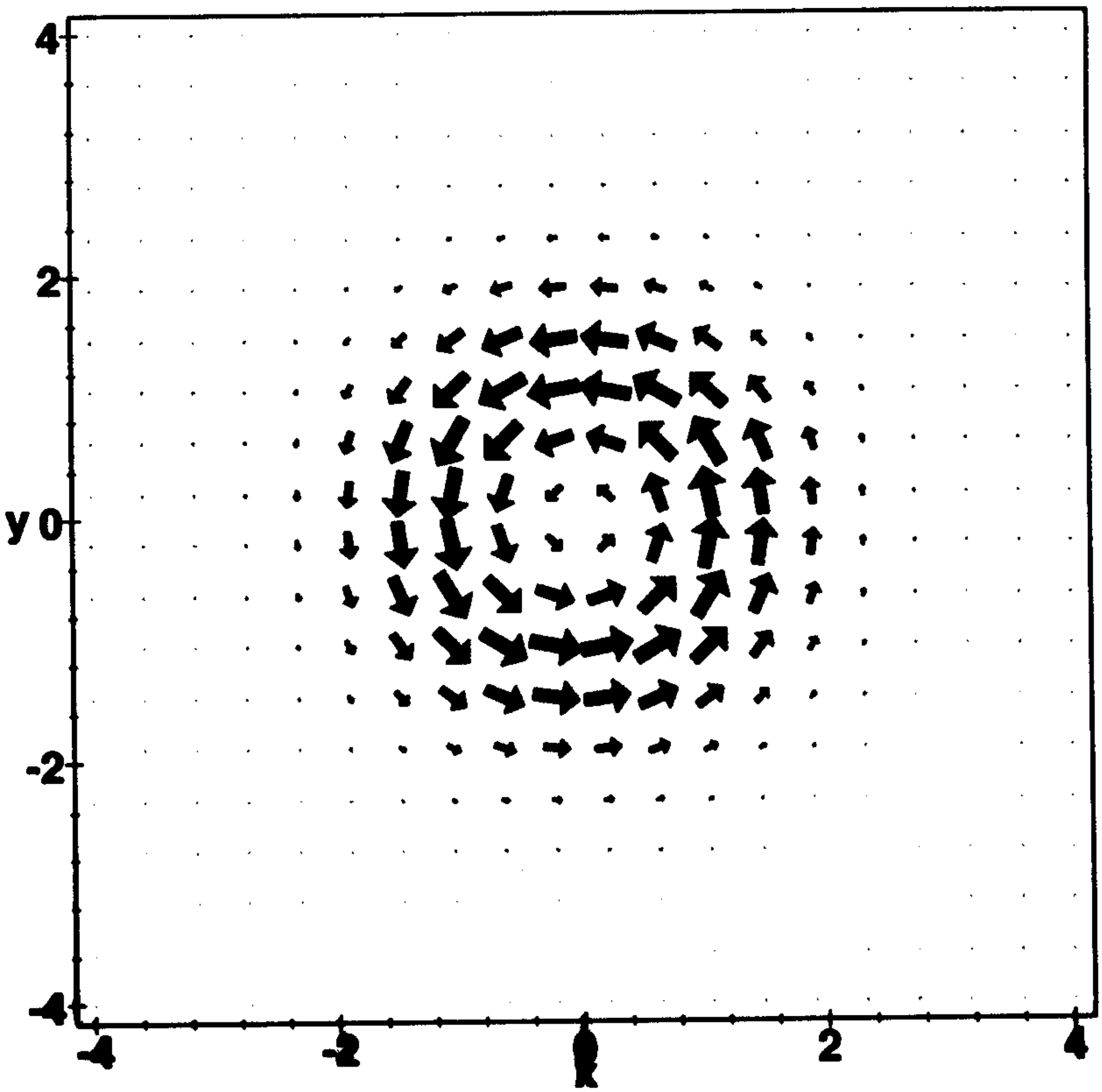
1-Teilchen-Spektrum

Quantendot-Wasserstoff

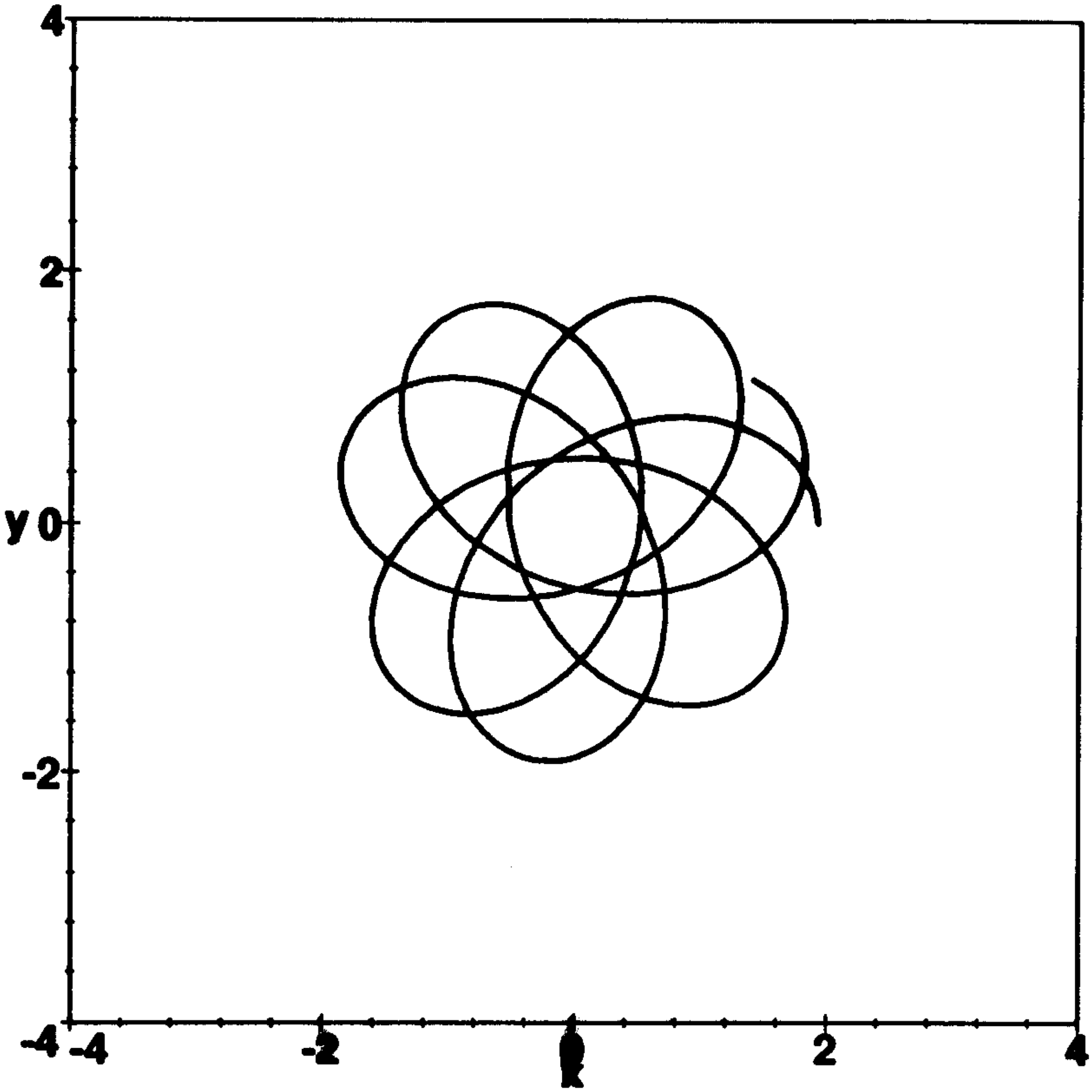



density, Np:= 0; Nm:= 1;
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-4
-2
0
2
4
xi

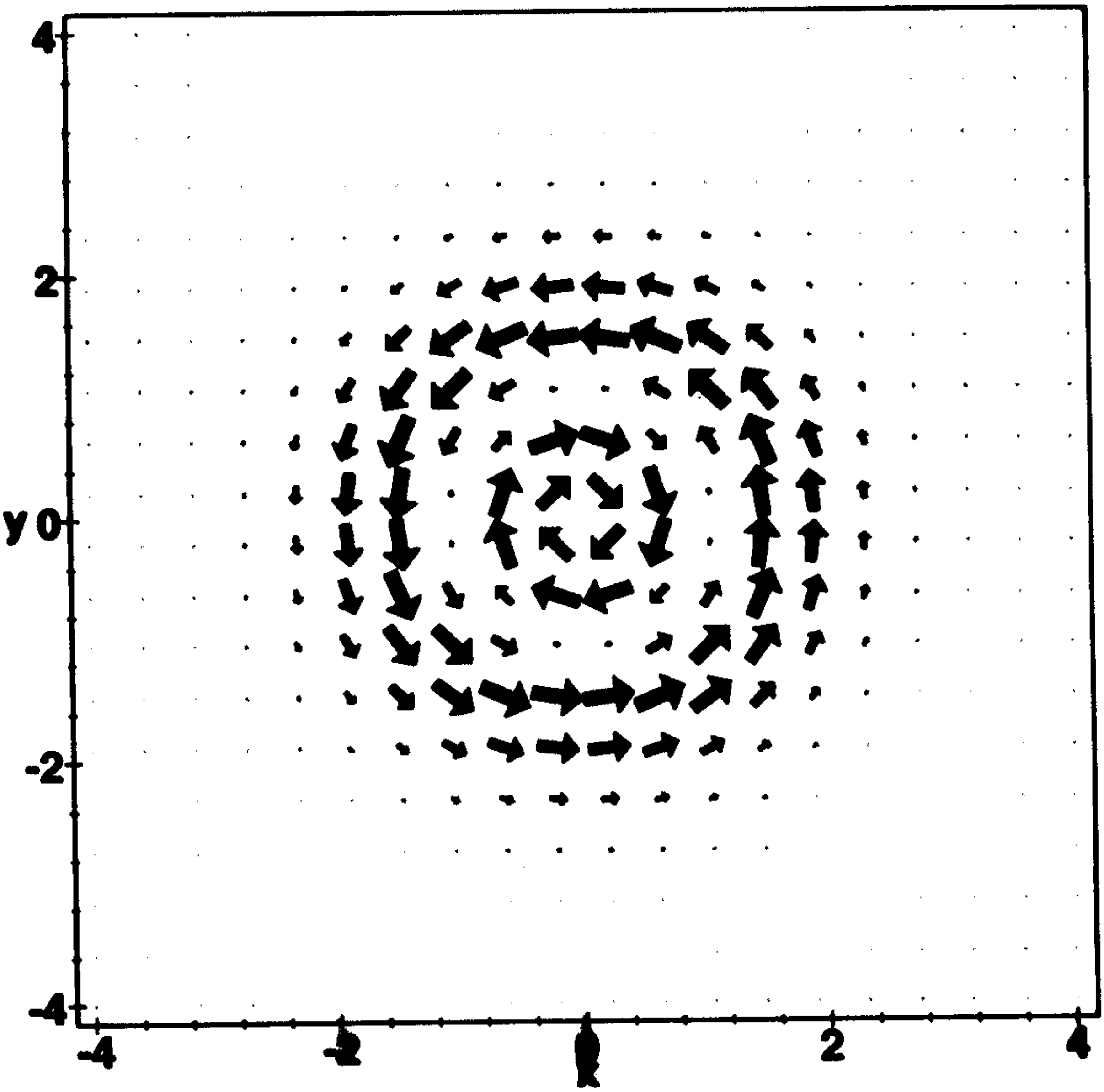
current density, Np:= 1; Nm:= 0; ratw:= 1;



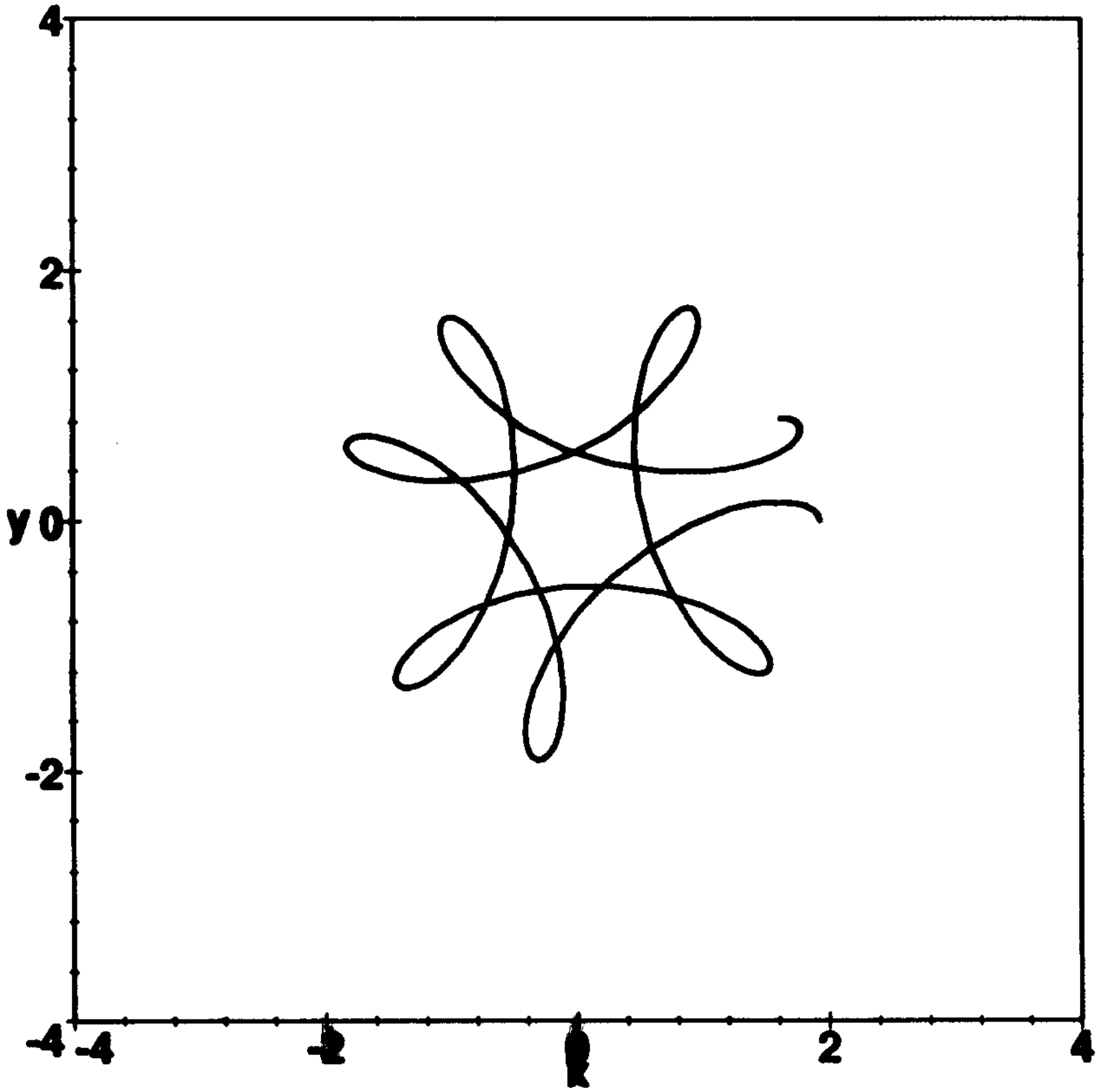
orbit, Np:= 1; Nm:= 0; ratw:= 1;



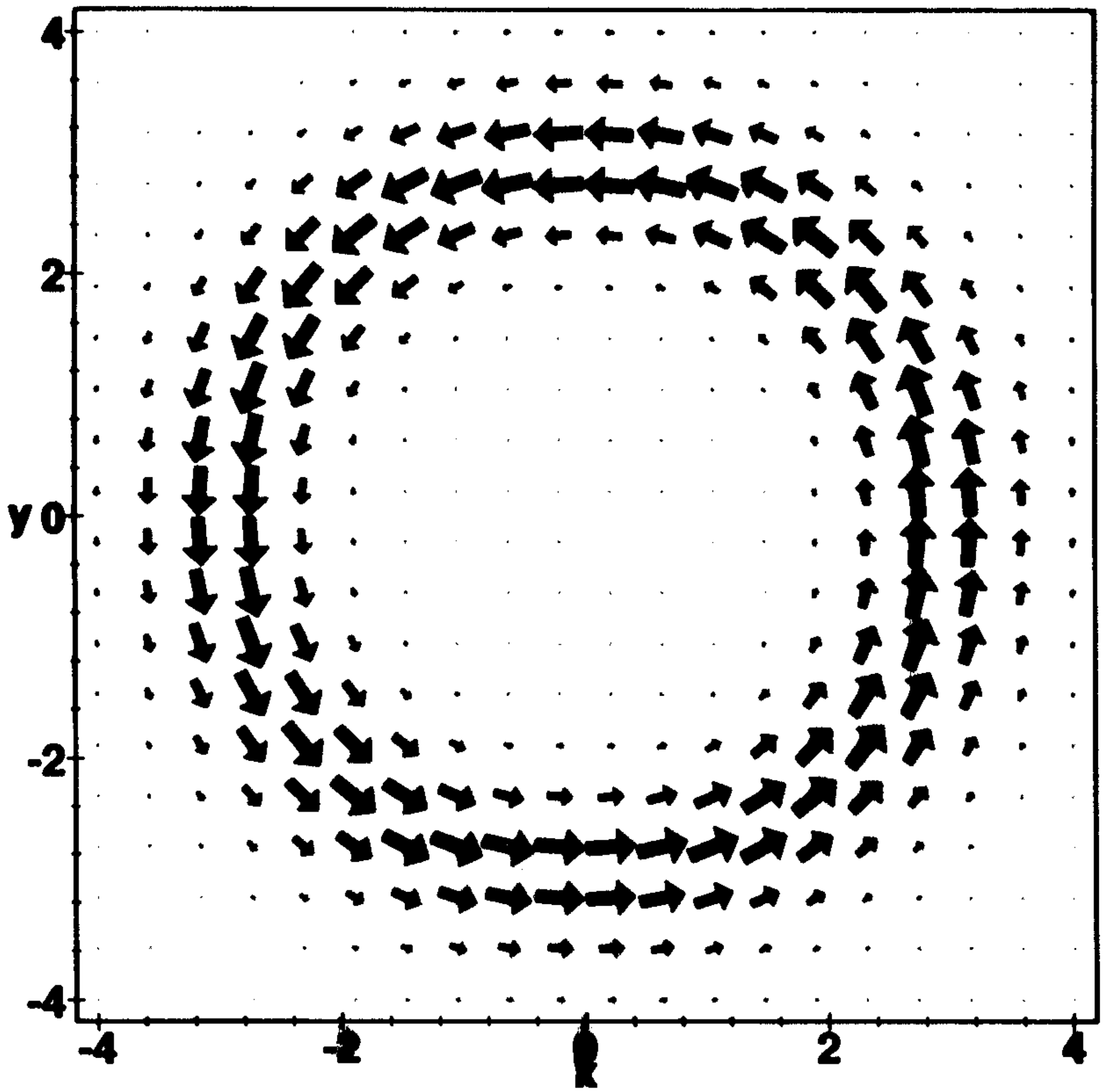
current density, Np:= 0; Nm:= 1; ratw:= 1;



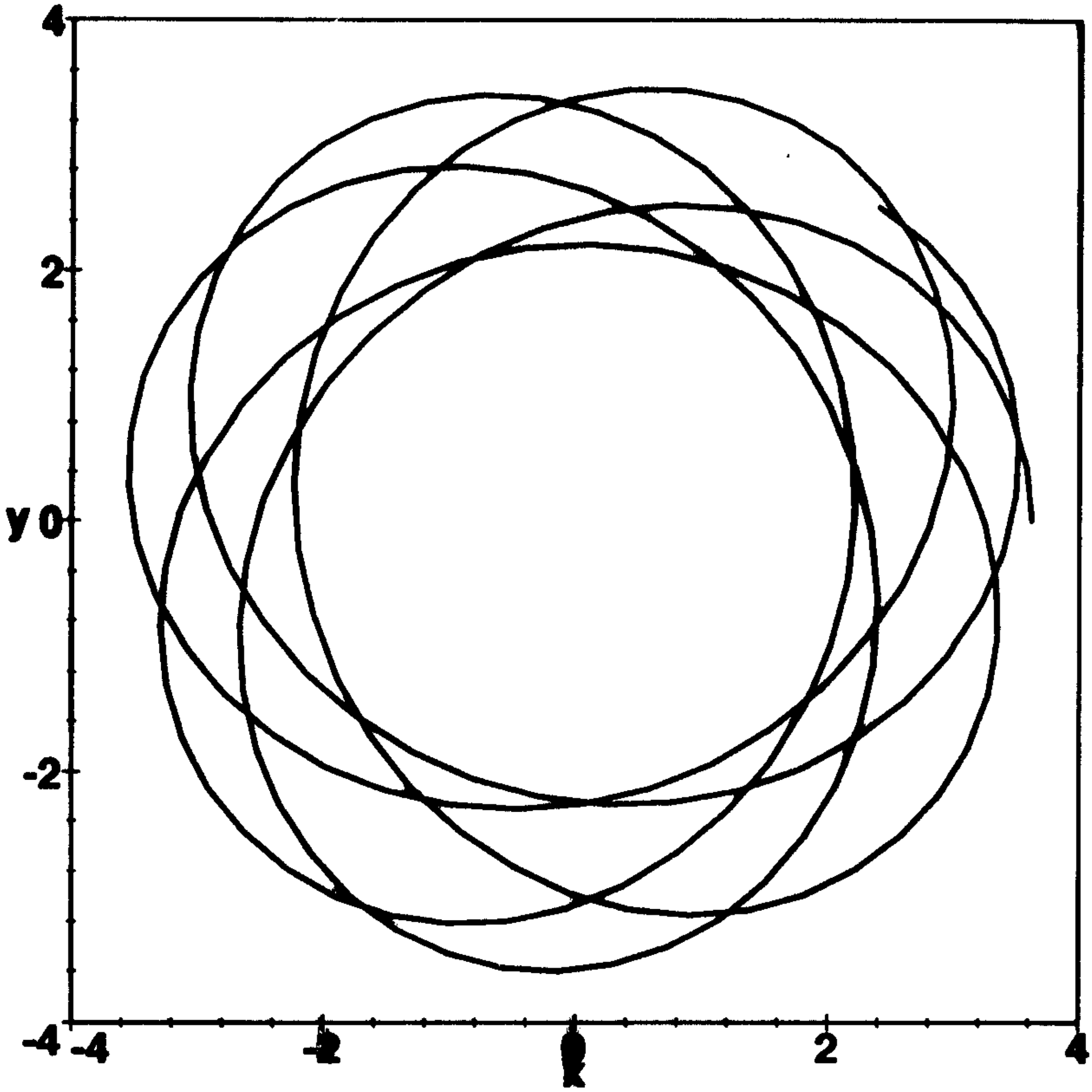
orbit, Np:= 0; Nm:= 1; ratw:= 1;



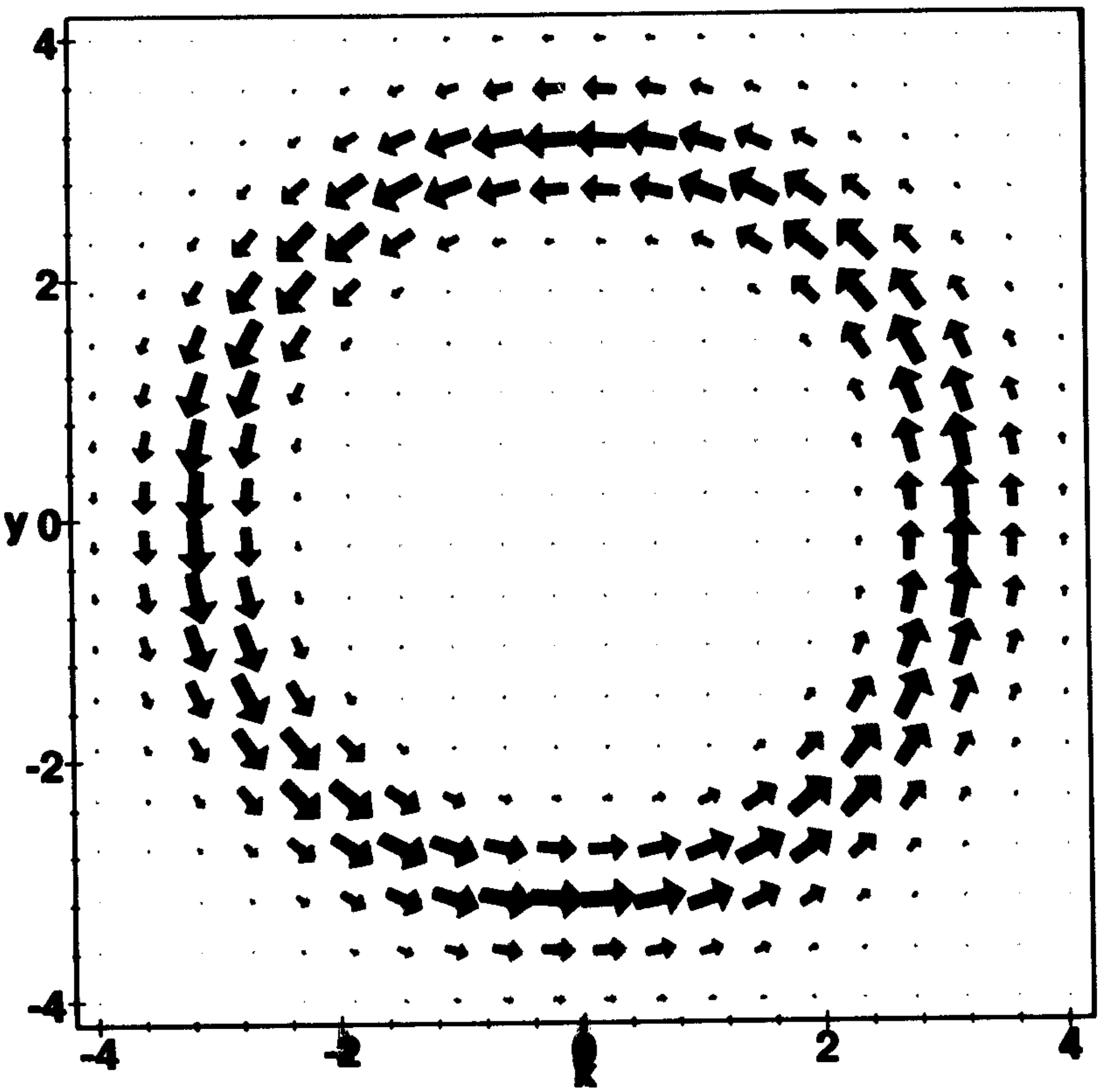
current density, Np:= 8; Nm:= 0; ratw:= 1;



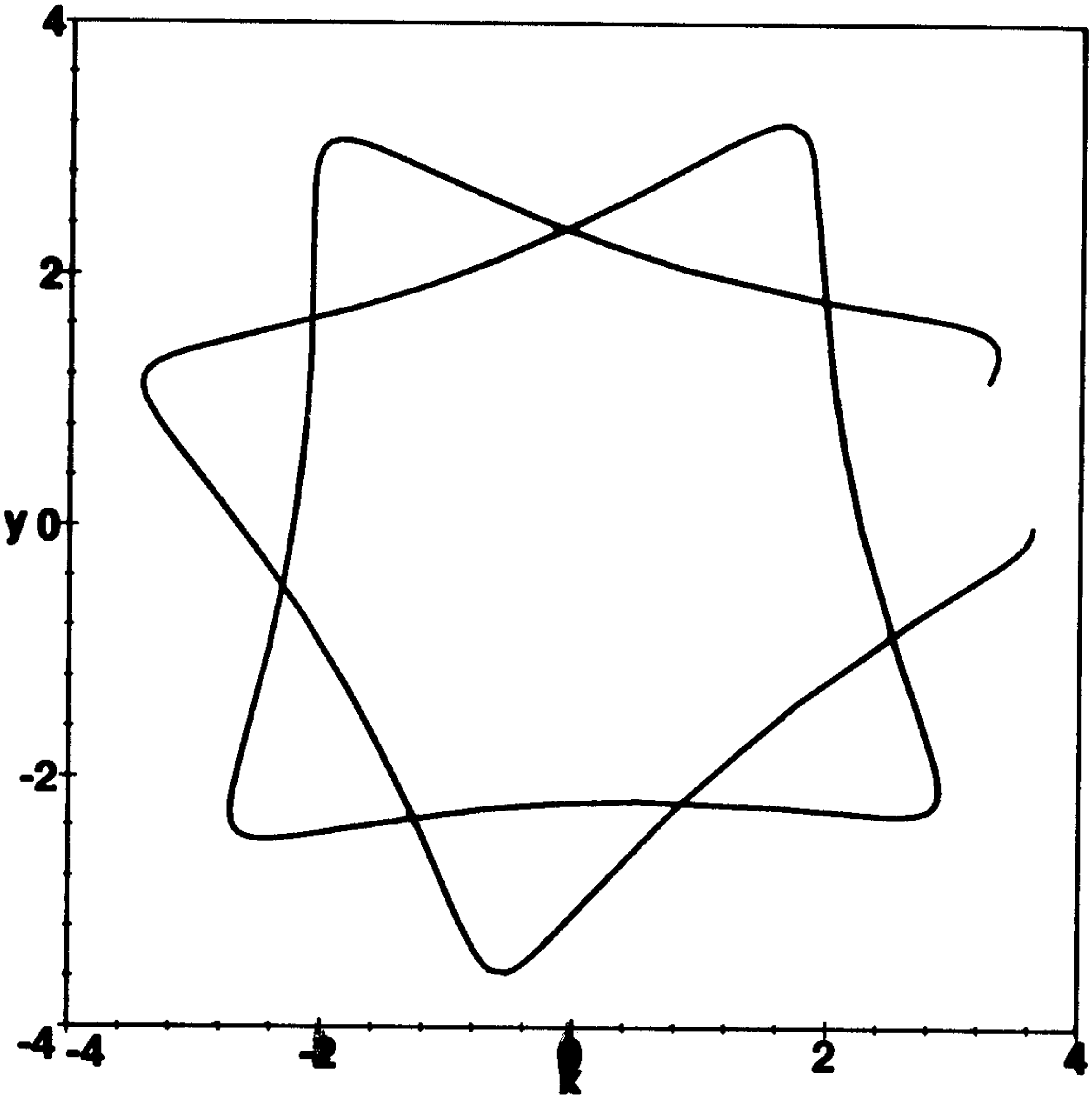
orbit, Np:= 8; Nm:= 0; ratw:= 1;



current density, Np:= 0; Nm:= 8; ratw:= 1;



orbit, Np:= 0; Nm:= 8; ratw:= 1;



QD-Helium

$$\mathcal{H} = H_0(1) + H_0(2) + \frac{e^2}{\epsilon|\vec{r}_1 - \vec{r}_2|}$$

couples motion of both particles

separation into center-of-mass and relative motion

$$\vec{R} = \tfrac{1}{2}(\vec{r}_1 + \vec{r}_2) \quad \vec{r} = \vec{r}_1 - \vec{r}_2$$
$$\vec{P} = \vec{p}_1 + \vec{p}_2 \quad \vec{p} = \frac{1}{2}(\vec{p}_1 - \vec{p}_2)$$

$$\mathcal{H} = H_0(\vec{R}, \vec{P}) + H_0(\vec{r}, \vec{p}) + \frac{e^2}{\epsilon r}$$

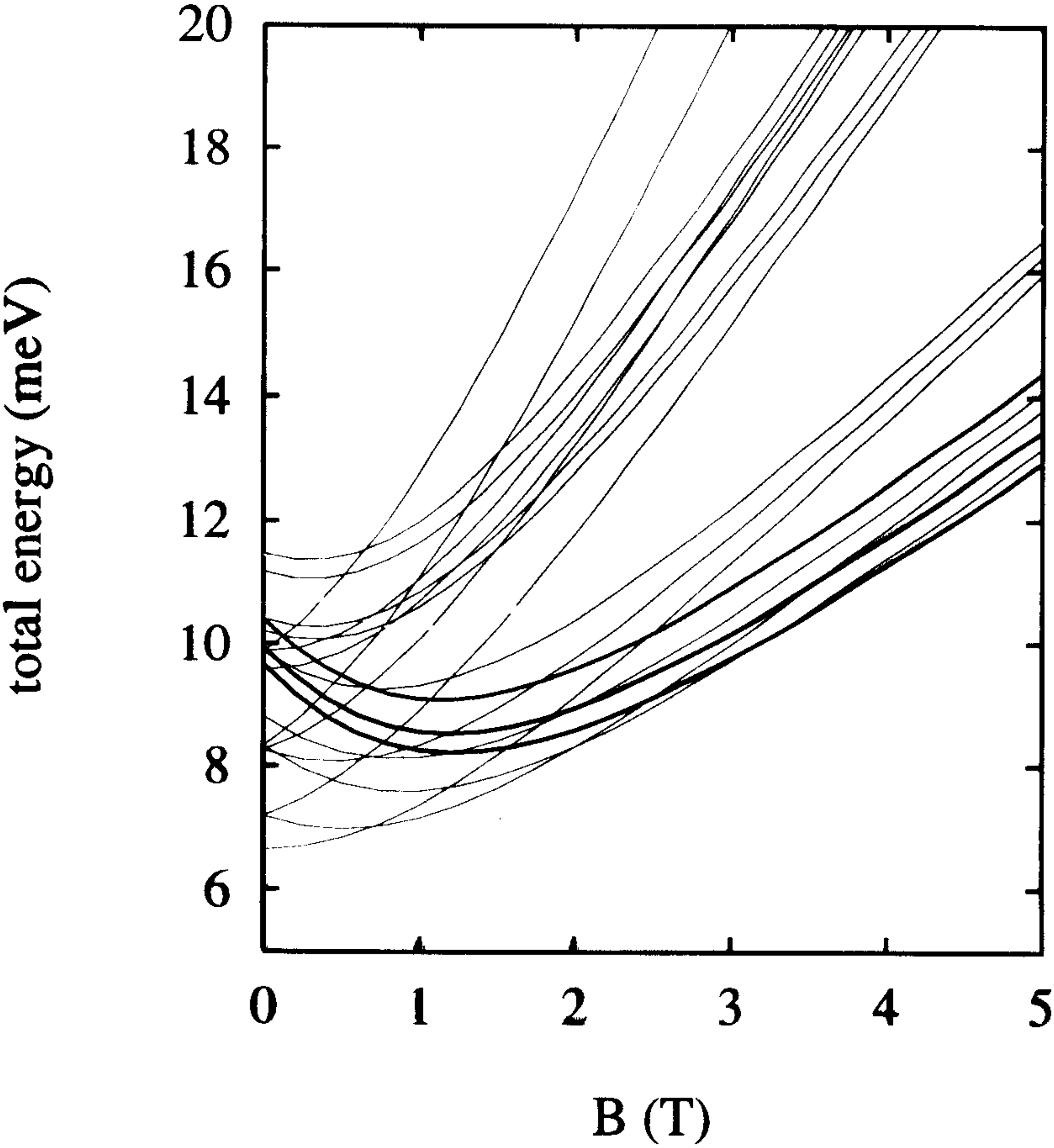
generalization for N particles:

$$\mathcal{H}_N = H(R_N, P_N) + \mathcal{H}_{N-1}(\vec{r}_i, \vec{p}_i)$$

Huser & Merkt,
Maksym & Chakraborty, ...

$\Rightarrow$ **generalized Kohn's Theorem for FIR spectroscopy**

Interacting Spectrum



Spin and Angular Momentum

$$|\Psi(1,2)\rangle = |\Phi_{CM}(1,2)\rangle|\phi_{rel}(1,2)\rangle\chi(S,S_z)$$

$$L_z^{rel}|\phi\rangle = \hbar M|\phi\rangle, \quad M = n_+ - n_-$$

Pauli-Principle: $P_{12}|\phi, chi\rangle = -|\phi, chi\rangle$

$$\begin{aligned} \langle\vec{r}|P_{12}|\phi,\chi\rangle &= \langle-\vec{r}|\phi,\chi\rangle \\ &= \langle\vec{r}|e^{iL_z\pi/\hbar}|\phi,\chi\rangle \end{aligned} \quad (1)$$

$\Rightarrow$

M odd	$\rightarrow \chi = \chi(1, S_z)$	(Triplet)
M even	$\rightarrow \chi = \chi(0,0)$	(Singlet)

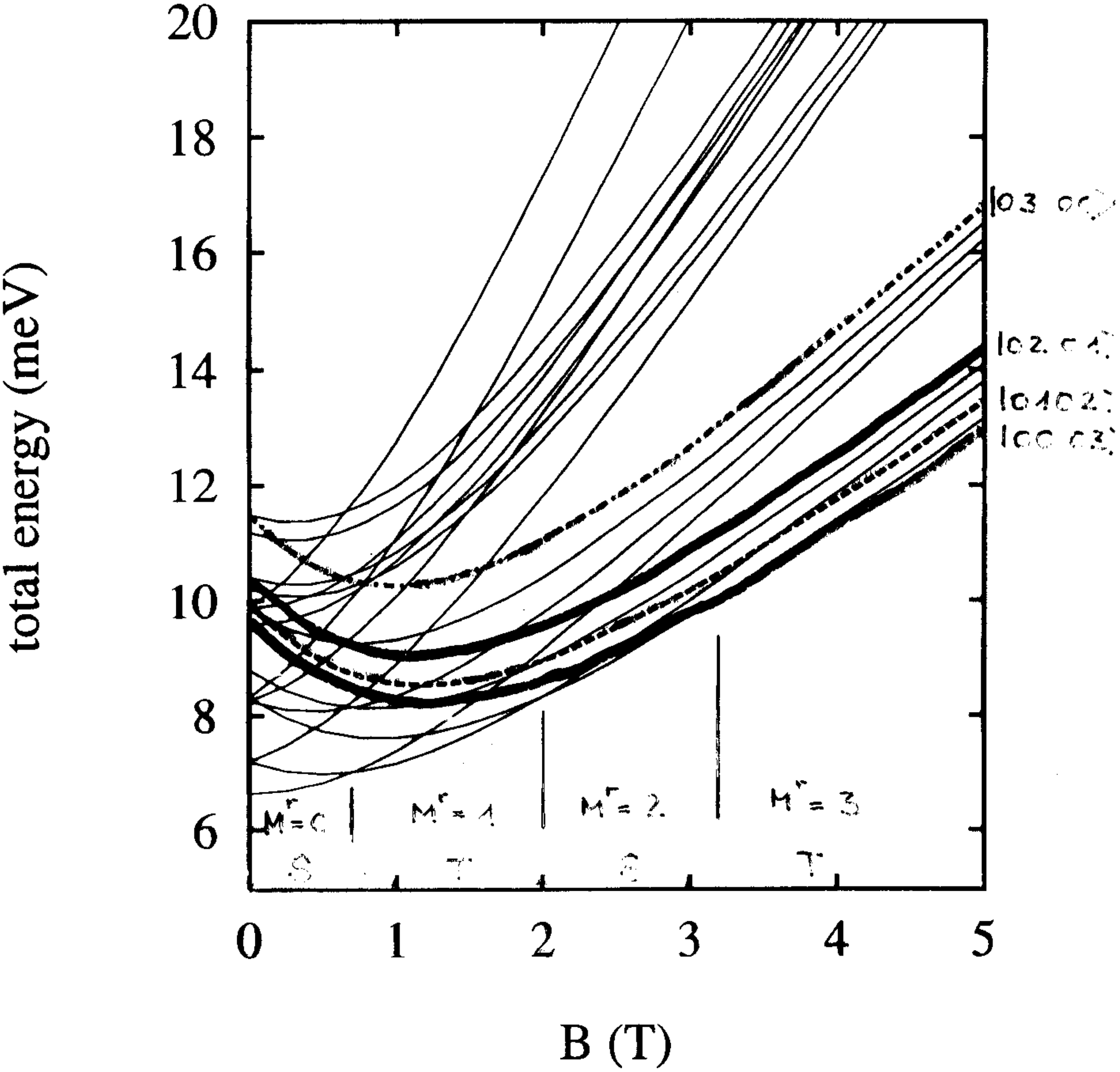
generalization for N electrons:

$$P_{ij}\vec{r}_m = e^{iL_z\alpha_{ijm}/\hbar}\vec{r}_n$$

for suitable relative coordinates

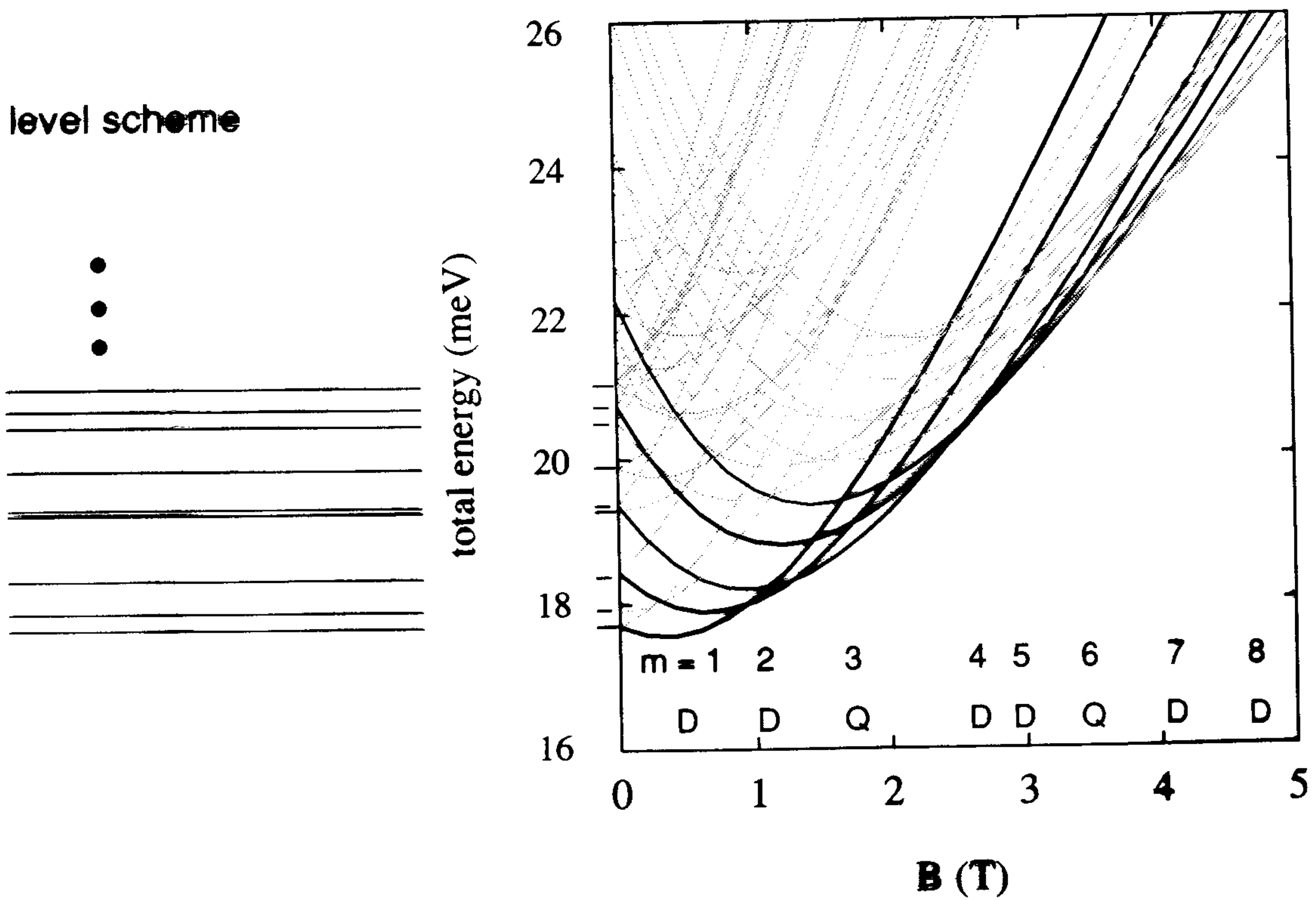
magic angular momentum quantum numbers

Interacting Spectrum



Spectrum of QD-Lithium

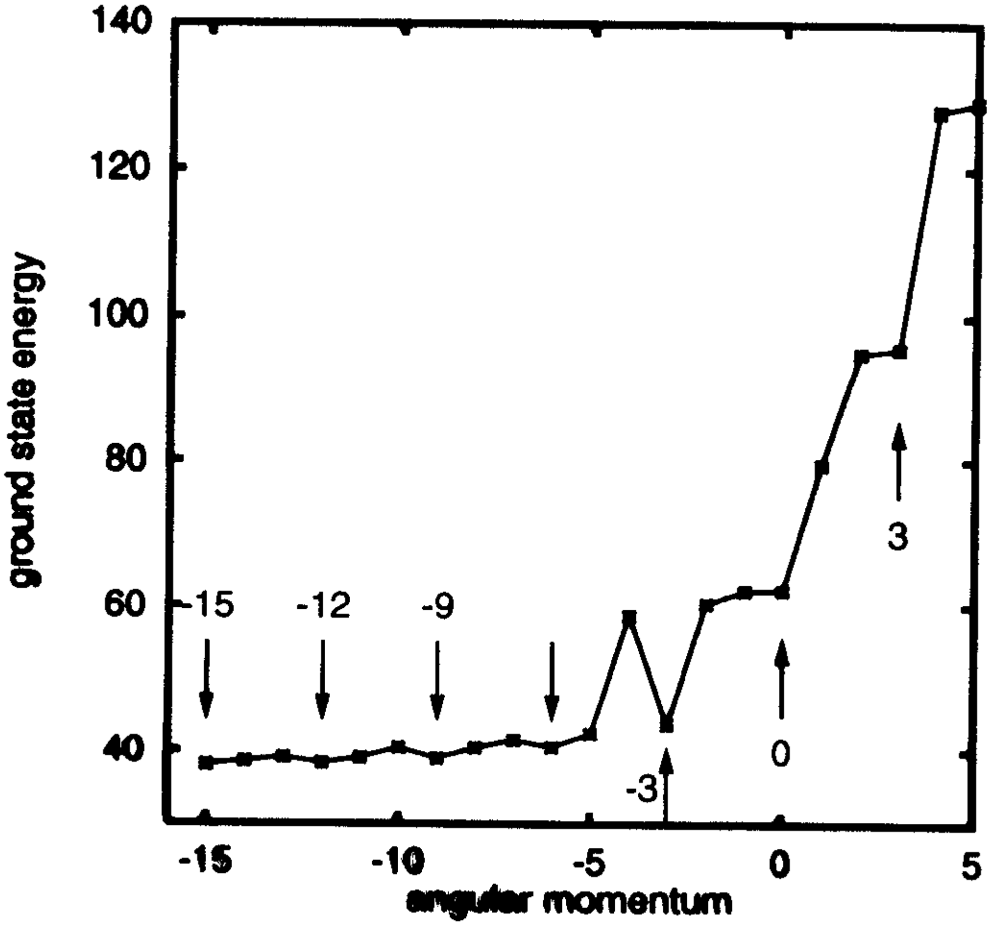
(3 electrons)



Magic Angular Momenta

Spin-polarized states occur

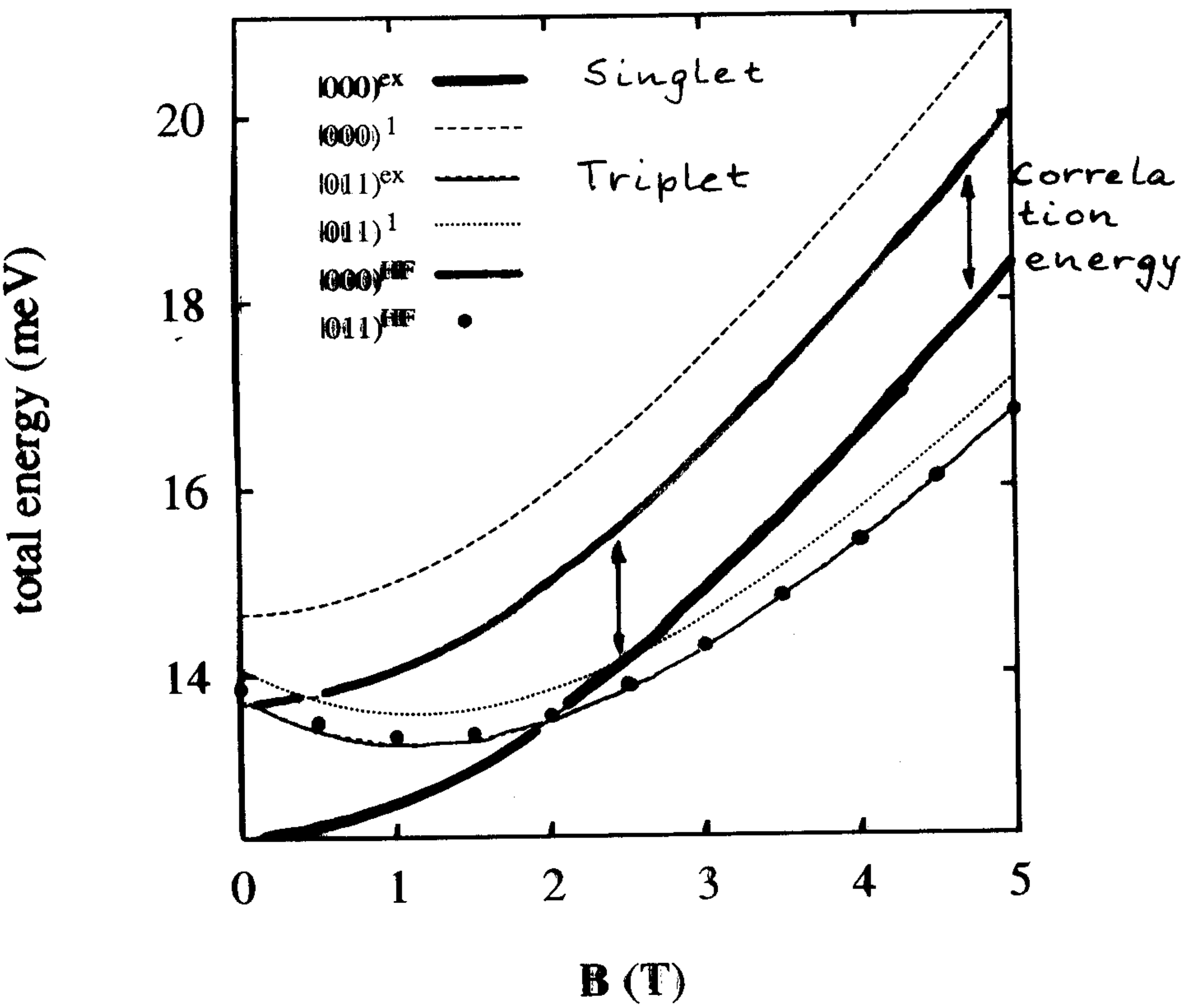
$$\text{for} \begin{array}{l} \text{QD-Helium} \\ \text{QD-Lithium} \\ \text{QD-Beryllium} \end{array} \Bigg\} \text{ at } L_z = \left\{ \begin{array}{l} 1, 3, 5, \ldots \\ 3, 6, 9, \ldots \\ 2, 6, 10, \ldots \end{array} \right.$$



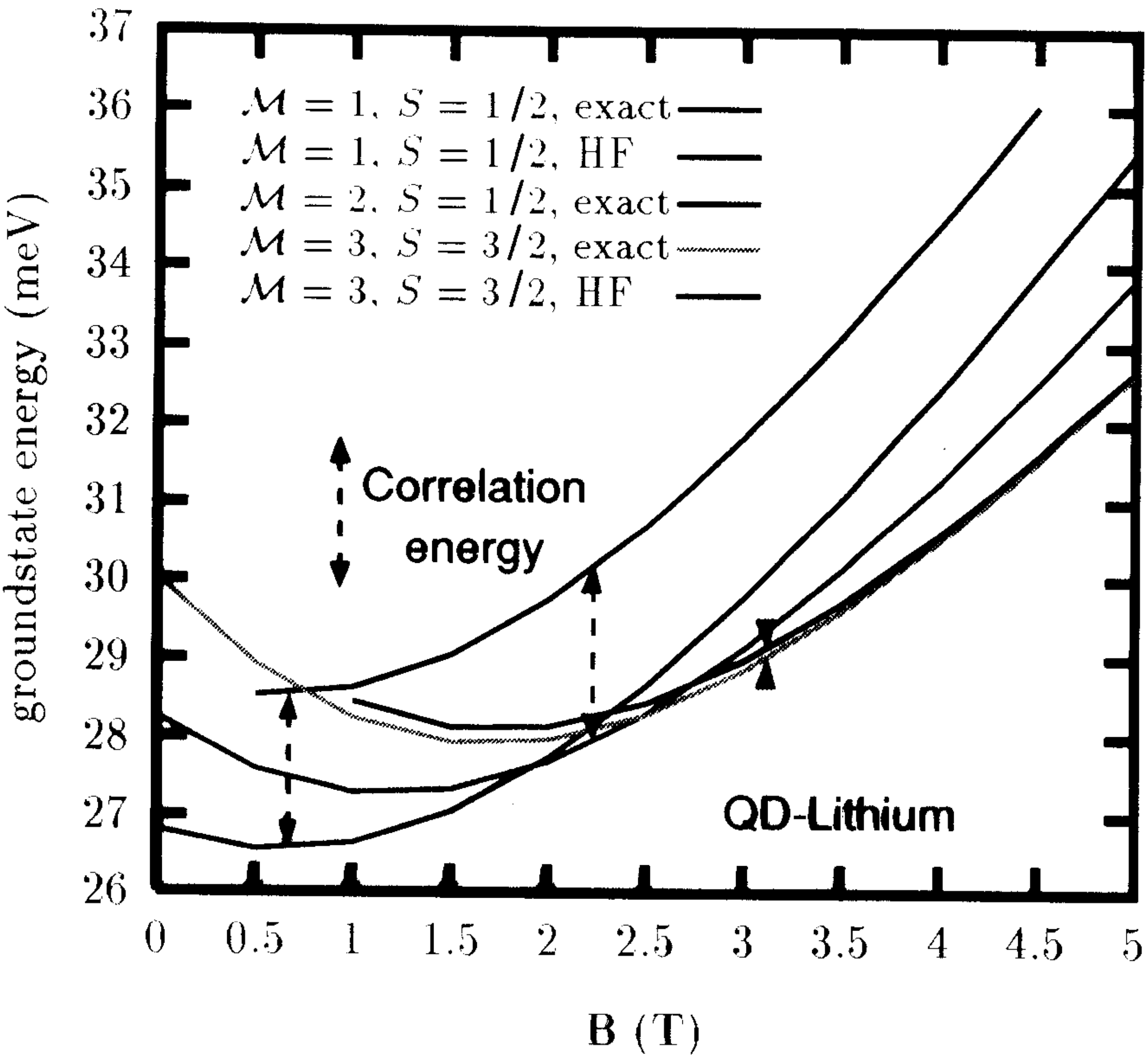
result from **Pauli-Principle and**
minimum energy vibrational modes

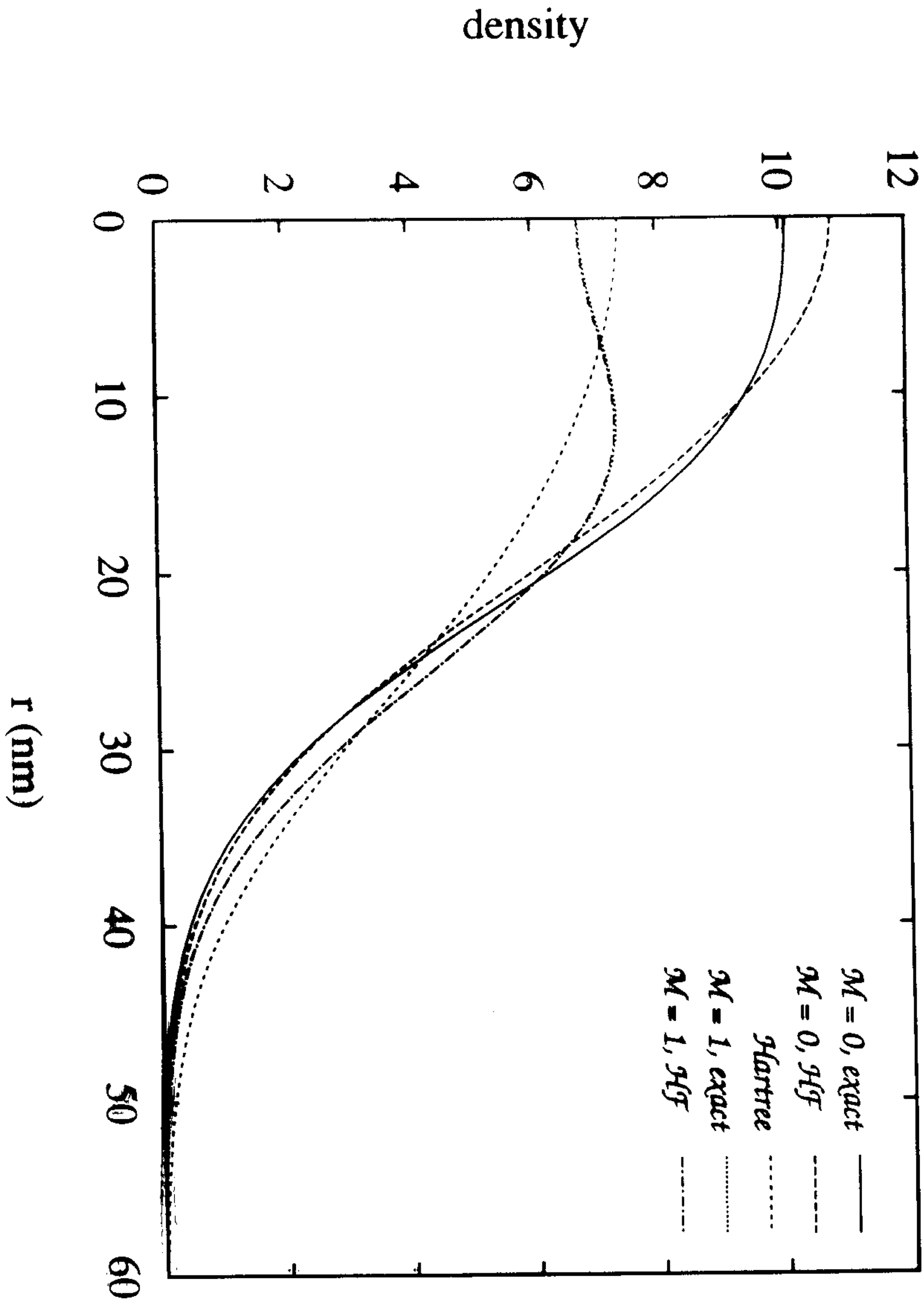
Maksym

Correlation Energy



Correlation Energy




density
r (nm)
0
2
4
6
8
10
12
0
10
20
30
40
50
60
$\mathcal{M} = 0$, exact
$\mathcal{M} = 0$, $\mathcal{HF}$
$\mathcal{H}$artree
$\mathcal{M} = 1$, exact
$\mathcal{M} = 1$, $\mathcal{HF}$

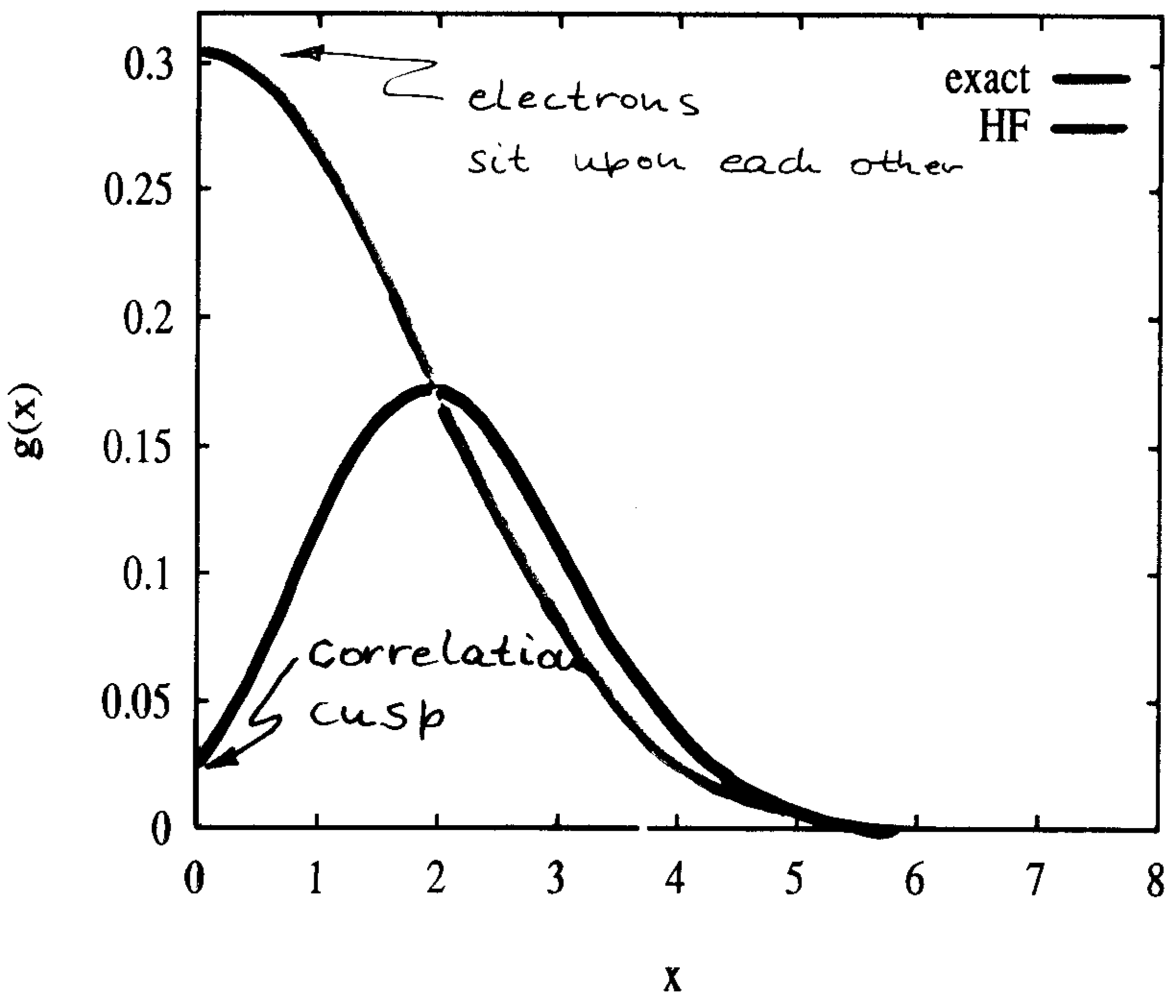
Pair-Correlation Function

why is the HF singlet energy that high?

Probability, for the electrons to be a distance r apart from each other

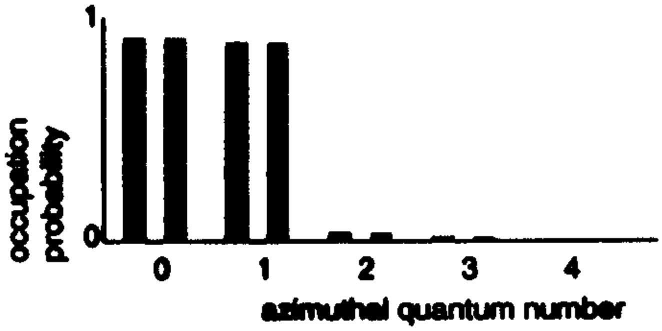
$$g(r) \propto \langle \delta(\vec{r} - (\hat{\vec{r}}_1 - \hat{\vec{r}}_2)) \rangle$$

$$\propto |\langle r | \tilde{0}^{rel} 0^{rel} \rangle|^2$$

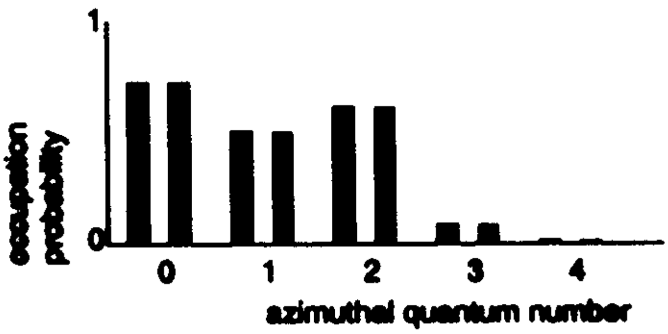


Wave Functions

uncorrelated 4-electron-state:



strongly correlated **4-electron-state:**



Figures from J. Palacios ***et al.***,
Superlattices and **Microstructures, 15**, 91, (1994)

strongly correlated states:
many single-particle states participate

Level Statistics

distribution of level spacing indicative of chaos in quantum systems

generic probability for finding 'nearest neighbor' level spacing s:

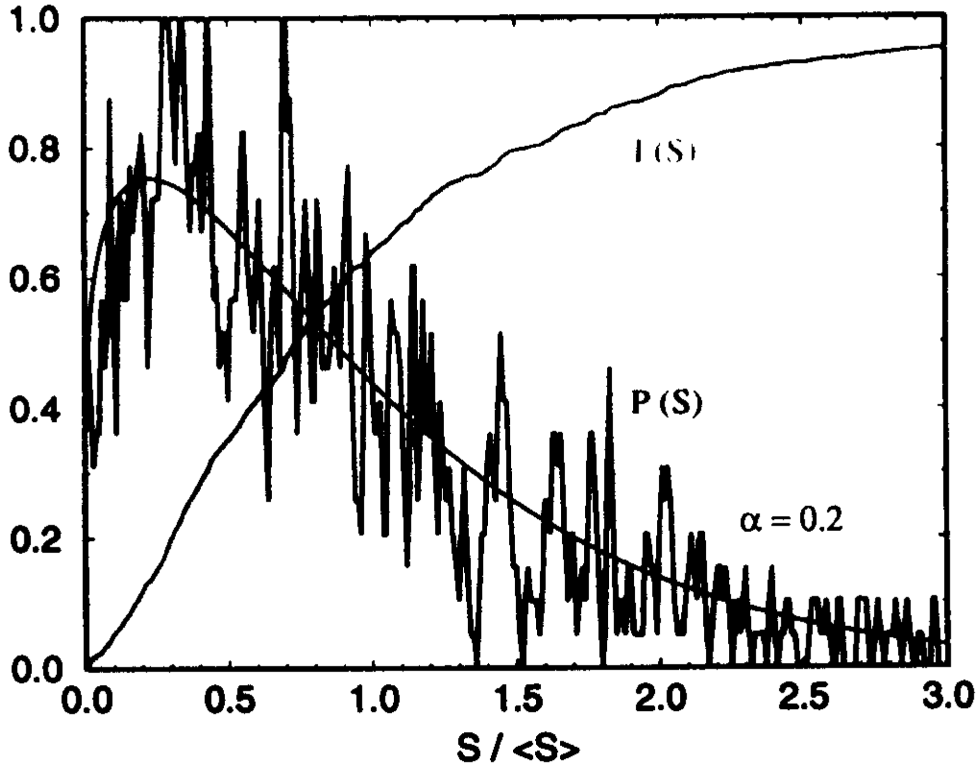
$$P(s) \propto \begin{cases} e^{-s/\langle s\rangle} & \text{Poisson} \quad \text{regular} \\ s e^{-s^2/\langle s\rangle^2} & \text{GOE} \quad \text{chaotic, B=0} \\ s^2 e^{-s^2/\langle s\rangle^2} & \text{GUE} \quad \text{chaotic, } B \neq 0 \end{cases}$$

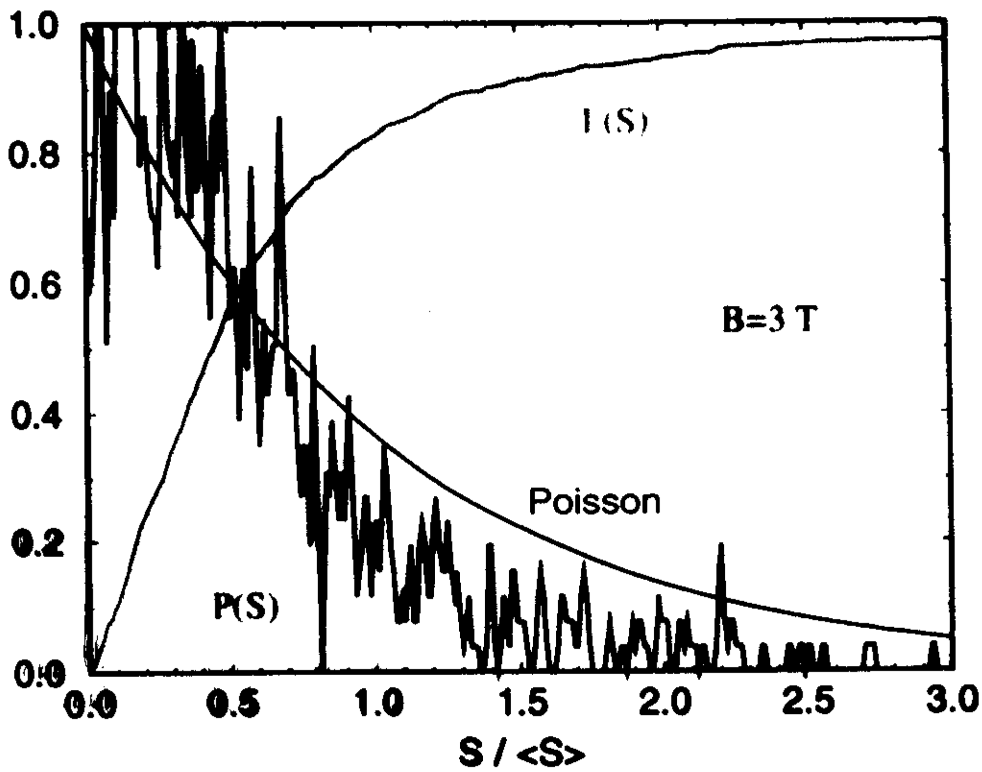
consequence of reduced symmetries

phenomenological interpolation formula:
Brody function $\quad P_\alpha(s) \propto s^\alpha e^{-\beta_\alpha s^{\alpha+1}}$

$\alpha = 0 \rightarrow$ Poisson
$\alpha = 1 \rightarrow$ GOE

From Chaos to Regular behavior





Summary

- Coulomb interaction
  - fine structure
  - magic numbers
  - correlations

- Correlations
  - strong in partially spin-polarized states
  - weak in fully spin-polarized states

- chaos by interaction
  oscillator localization vs Coulomb repulsion