# Models of quantum dots


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## Cooperation

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*Not a report on the history of dot models*

## Dimensionality + Shape

2D ↔ 3D

Etched + Gate defined ↔ Self-assembled

Ratio between width, thickness, and $\lambda_F$

- A. Kumar and S. E. Laux and F. Stern, Phys. Rev. B**42**, 5166 (1990)
- Experiment + models
- Parabolic confinement + small deviations
- Almost circular
- Commonly: Coulomb Energy ∼ confinement energy



## Noninteracting confined Electrons

- Parabolic confinement, $\mathbf{B} = B\hat{\mathbf{z}}$

Hamiltonian of a single electron

$$\hat{H}^0 = \frac{1}{2m^*}\left(\hat{\mathbf{p}} + \frac{e}{c}\hat{\mathbf{A}}(\mathbf{r})\right)^2 + \frac{1}{2}m^*\omega_0^2\hat{r}^2$$

Wave functions

$$\phi_{M,n_r}(r,\phi) = \frac{1}{2^{\frac{|M|+1}{2}}a}\left(\frac{n_r!}{\pi(|M|+n_r)!}\right)^{\frac{1}{2}}\left(\frac{r}{a}\right)^{|M|} \times e^{-r^2/4a^2} L_{n_r}^{|M|}\left(\frac{r^2}{2a^2}\right)e^{-iM\phi}$$

Natural length scale

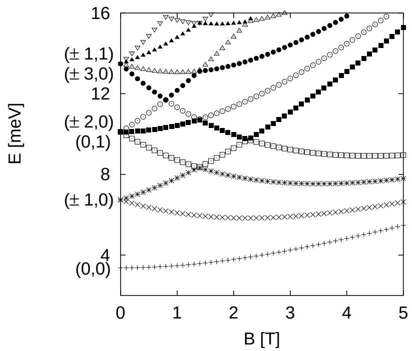
$$a^2 = \frac{\ell^2}{\sqrt{1+4(\frac{\omega_0}{\omega_c})^2}}, \quad \ell = \sqrt{\frac{\hbar c}{eB}}, \quad \omega_c = \frac{eB}{m^* c}$$

Single-electron energy spectrum

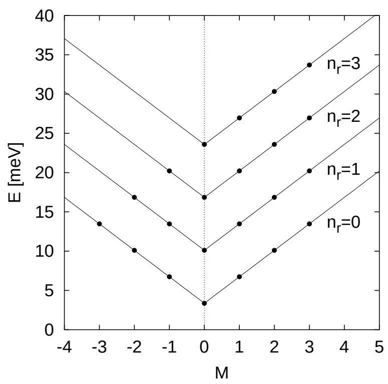
$$E_{M,n_r} = (n_r + \frac{|M|}{2} + \frac{1}{2})\hbar(\omega_c^2 + 4\omega_0^2)^{\frac{1}{2}} - \frac{1}{2}M\hbar\omega_c.$$

- V. Fock, Z. Phys. **47**, 446 (1928)
- C. G. Darwin, Proc. Camb. Phil. Soc. **27**, 86 (1930)

## Darwin-Fock single-electron energy spectrum

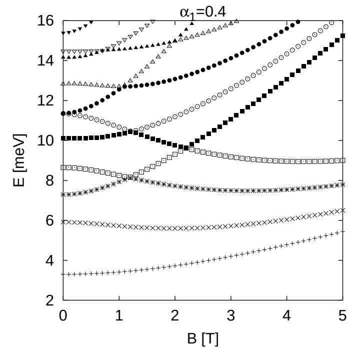



B=0 T, (circular dot), ($\hbar\omega_0 = 3.37$ meV)

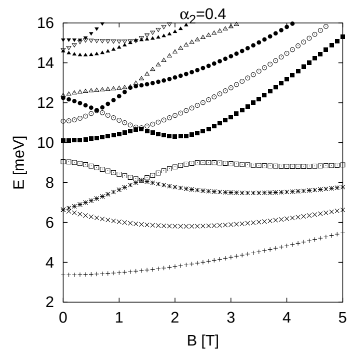





## Elliptic deviation, (dipole)




## Square deviation, (quadrupole)



## Exact numerical diagonalization

Many-electron Hamiltonian

$$\hat{H} = \sum_{i=1}^{N} (\hat{T}_i + \hat{U}_i) + \frac{1}{2} \sum_{\substack{i,i=1 \\ i \neq i}}^{N} \hat{V}_{i,j}$$

$\Downarrow$

Matrix elements of $\hat{H}$

in a truncated many-electron basis $||\Theta\rangle$

(made from the single electron states $|M, n_r\rangle$ ($\sim \phi_{M,n_r}$))

$\Downarrow$

Interacting many-electron states $||\Theta)$

and energy spectrum $E_\Theta$

$||\Theta) = ||j, \mathcal{M}, \mathcal{S})$

$j$: number of state

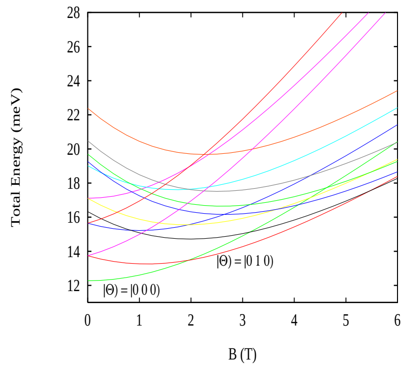
$\mathcal{M}$: quantum number of total angular momentum

$\mathcal{S}$: quantum number of total spin



- Transformation to center-of-mass (cm.) and relative motion (rel.) coordinates
- Successful, few electrons

Few lowest two-electron states

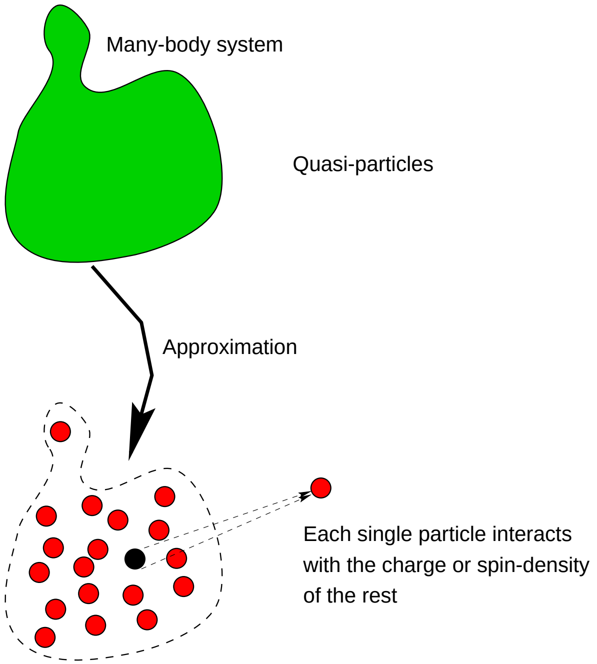



Succession of ground states

- P. A. Maksym and T. Chakraborty, Phys. Rev. Lett. **65**, 108 (1990)
- D. Pfannkuche, V. Gudmundsson, and P. Maksym, Phys. Rev. B**47**, 2244 (1993)

## Mean field approaches

More electrons, larger dots




$$+E_{\text{corr}}$$



## Hartree-Fock approximation

Variational ansatz

$$\hat{H} = \sum_{i=1}^{N} (\hat{T}_i + \hat{U}_i) + \frac{1}{2} \sum_{\substack{i,i=1 \\ i \neq i}}^{N} \hat{V}_{i,j}$$

$$\downarrow$$

$$\text{assume: } \Phi = \frac{1}{\sqrt{N!}} \det[\phi_i(x_j)]$$

$$\downarrow$$

$$\hat{H}_{HF} = \sum_{i=1}^{N} \hat{h}_{HF}^{(i)} = \sum_{i=1}^{N} (\hat{T}_i + \hat{U}_i + \hat{V}_{HF}^{(i)})$$

## HF-equations

$$\{H_0 + U_{conf}(\mathbf{r}) + V_H(\mathbf{r})\}\psi_\alpha(\mathbf{r}) - \int d\mathbf{r}' \Delta(\mathbf{r},\mathbf{r}')\psi_\alpha(\mathbf{r}') = \epsilon_\alpha \psi_\alpha(\mathbf{r})$$

$$V_H(r) = \frac{e^2}{\kappa}\int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$\Delta(\mathbf{r},\mathbf{r}') = \frac{e^2}{\kappa}\sum_\beta f(\epsilon_\beta - \mu)\frac{\psi^*_\beta(\mathbf{r}')\psi_\beta(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}$$

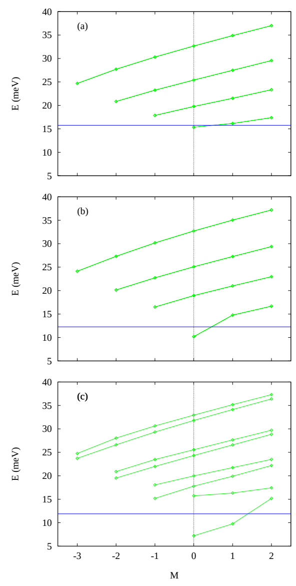
$$n(\mathbf{r}) = \sum_\alpha |\psi_\alpha(\mathbf{r})|^2 f(\epsilon_\alpha - \mu)$$

$$\int d\mathbf{r}'\, n(\mathbf{r}',\mu) = \text{const.}$$



## Two electrons

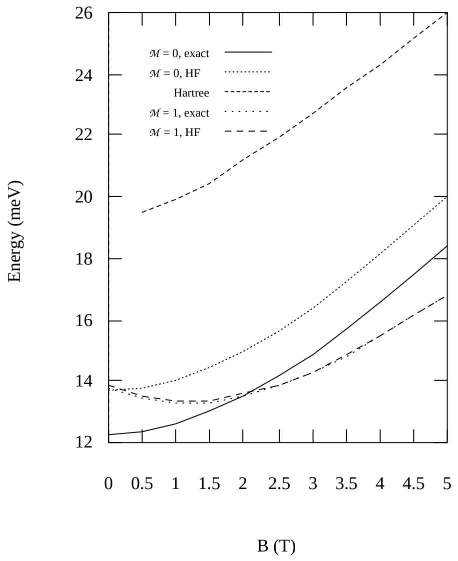
Hartree $\mathcal{S}=0$: (a)




Hartree-Fock $\mathcal{S}=0$: (b) , $\mathcal{S}=1$: (c)

Spin enhancement, exchange interaction

## Exchange is not always enough



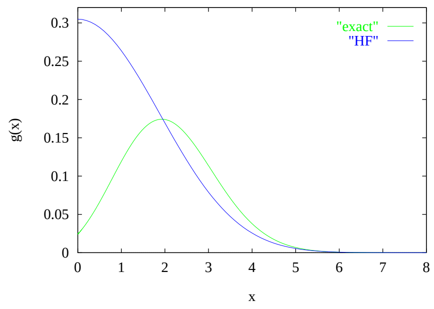

- D. Pfannkuche, V. Gudmundsson, and P. Maksym, Phys. Rev. B**47**, 2244 (1993)



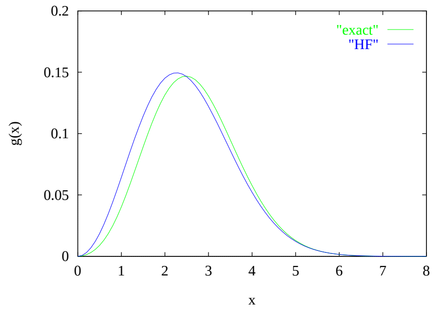
## Correlation

$$g(\mathbf{r}) = \frac{2\pi\lambda^2}{N(N-1)}\langle\sum_{i\neq j}\delta(\mathbf{r}-\mathbf{r}_i+\mathbf{r}_j)\rangle,$$

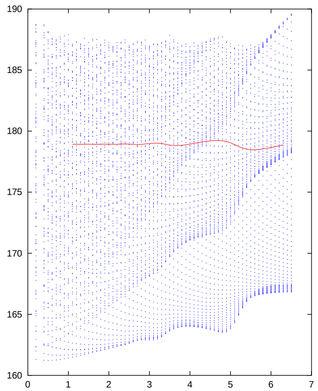
$\mathcal{M} = 0$



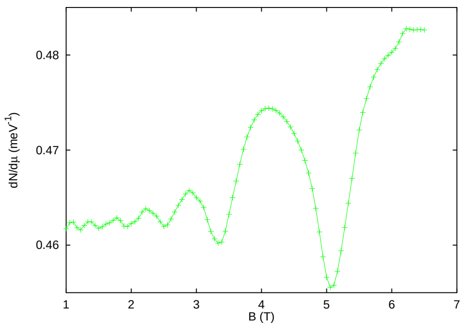

$\mathcal{M} = 1$



N=60, energy spectrum, T=1 K




Density of states (TDOS)






**Hartree:** $\rightarrow$ Unique ground state

**Hartree-Fock:** $\rightarrow$ Different end states

Example

2 electrons in a quantum dot:
Singlet $\mathcal{S} = 0$, triplet $\mathcal{S} = 1$

Restricted, unrestricted HF-approximation

Example Circular quantum dot, parabolic confinement

$\Downarrow$

$$[\hat{H}, \hat{L}^2] = [\hat{H}, \hat{L}_z] = 0 = [\hat{H}, \hat{S}^2] = [\hat{H}, \hat{S}_z]$$

$\Downarrow$

States labelled by $\alpha = (n, M, s)$

$\Downarrow$

Coulomb interaction mixes $n$, not $M$ and $s$

RHF

- $||\Phi\rangle$ and $|\psi_\alpha\rangle$ same symmetry as $\hat{H}$
- Single-particle states have either $s = \pm\frac{1}{2}$

UHF

- Broken symmetry ground state with lower energy
- States with no definite $s$
- Skyrmions
- Symmetry broken with initial state in iteration

Nonspherical atoms



Iteration

Numerical integration

or

Solution in a basis $\{\phi_\alpha\}$

**Basis:** For example eigenstates of
$H_0\phi_\alpha = E_0\phi_\alpha$, Fourier basis, ...

**Matrix elements:** $\langle\alpha|U|\beta\rangle, \ldots,$ singularity,
CPU size and speed, mapping:
$\alpha = (n, M, s) \rightarrow i, \ldots$

**Convenient basis:** Matrix elements,
convergence, ...

Convergence

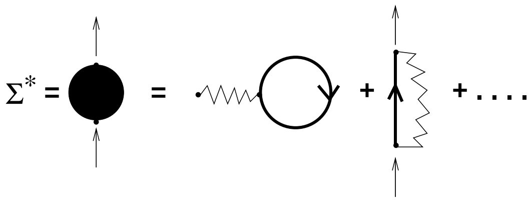
**Slow mixing:**

$$n_s^i(\mathbf{r}) \leftarrow \delta \cdot n_s^i(\mathbf{r}) + (1-\delta) \cdot n_s^{i-1}(\mathbf{r})$$

## General

Pure state $v$-representability

- Not all states can be represented by a Slater determinant
- Degenerate states $||\Phi\rangle$
- Example, FQHE in a homogeneous system
- Ordering, correlation

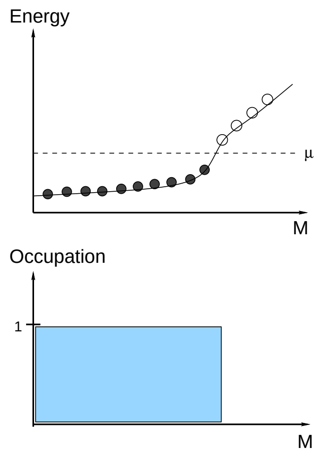



- O. Heinonen, M. I. Lubin, and M. D. Johnson, Phys. Rev. L **75**, 4110 (1995)



## Maximum Density Droplet (MDD)

High B, large dot




Other phases possible

- A. H. MacDonald, S. R. Eric Yang, and M. D. Jonson, Aust. J. of Phys. **46**, 345 (1993)
- Maximum-Density Droplet and Charge Redistributions in Quantum Dots at High Magnetic Fields, T. H. Oosterkamp, J. W. Janssen, L. P. Kouwenhoven, D. G. Austing, T. Honda et al. Physical Review Letters, Volume 82, Issue 14, pp. 2931-2934

## Other phases possible

- Hund's Rules and Spin Density Waves in Quantum Dots, M. Koskinen, M. Manninen, S. M. Reimann Phys. Rev. Lett. **79**, 1389 (1997)
- Quantum dots in magnetic fields: Phase diagram and broken symmetry of the Chamon-Wen edge, S. M. Reimann, M. Koskinen, M. Manninen, B. R. Mottelson cond-mat/9904067
- V. Gudmundsson and J. J. Palacios, Phys. Rev. B**52**, 11266 (1995)
- Skyrmions and the crossover from the integer to fractional quantum Hall effect at small Zeeman energies, S. L. Sondhi, A. Karlhede, and S. A. Kivelson, E. H. Rezayi, Phys. Rev. B**47**, 16419 (1993)
- Phase transitions in quantum dots, H.-M. Müller and S. E. Koonin, Phys. Rev. B **54**, 14532 (1996)

HFA, UHFA $\leftarrow$ model of exchange effects

$\rightarrow$ DFT$\cdots$



## DFT

## CSDFT

$$\begin{aligned} E &= \sum_{iM\sigma}^{N} \epsilon_{iM\sigma} - \frac{e^2}{2\kappa}\int d\mathbf{r}d\mathbf{r}'\frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \\ &- \sum_{\sigma}\int d\mathbf{r} n_\sigma(\mathbf{r})V_{xc\sigma}(\mathbf{r}) \\ &- \frac{e}{c}\int d\mathbf{r}\mathbf{j}_p(\mathbf{r})\cdot\mathbf{A}_{xc}(\mathbf{r}) + E_{xc}[n,\xi,\mathcal{V}] \end{aligned}$$

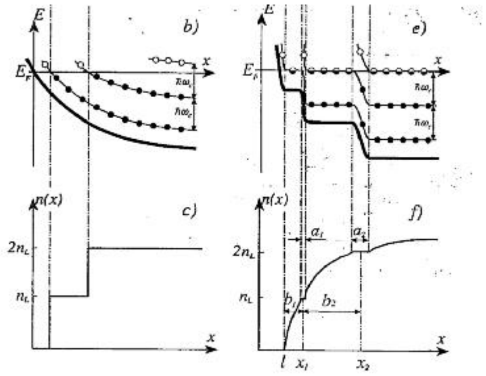
- Current-density-functional theory of quantum dots in a magnetic field M. Ferconi and G. Vignale, Phys. Rev. B**50**, 14722 (1994)

## Extensions

- Correlated ground states with (spontaneously) broken time-reversal symmetry, Behnam Farid, cond-mat/9604138
- GW + $\cdots$

## Large Systems

### Compressible - incompressible regions




- Electrostatics of edge channels, D. B. Chklovskii, B. I. Shklovskii, and L. I. Glazman, Phys. Rev. B**46** 4026 (1992)



### Hydrodynamic models

- Magnetoplasmons in a two-dimensional electron fluid: Disk geometry, A. L. Fetter, Phys. Rev. B**33**, 5221 (1986)

- Magnetoplasma excitations in anharmonic electron dots, Z. L. Ye and E. Zaremba, Phys. Rev. B**50** 17217 (1994)

### Thomas-Fermi

- Ground states of large quantum dots in magnetic fields E. H. Lieb, J. P. Solovej, and J. Yngvason Phys. Rev. B**51**, 10646 (1995)

### Monte-Carlo

## FIR-absorption

### Kohns theorem

- FIR-field with $\lambda >> $ dot size
- Parabolic confinement
- FIR-field couples only cm. coordinates
- Absorption independent of N

$$\mathcal{H}^{rad} = \sum_{i=1}^{N} e\mathcal{E}^{ext} \cdot \mathbf{r} e^{i\omega t} = eN\mathbf{R} \cdot \mathcal{E}^{ext} e^{i\omega t}$$


- P. Bakshi, D. Broido, and K. Kempa, Phys. Rev. B**42**, 7416 (1990)
- P. A. Maksym and T. Chakraborty, Phys. Rev. Lett. **65**, 108 (1990)


### Exact numerical diagonalization

Oscillator strength, ground state → excited state

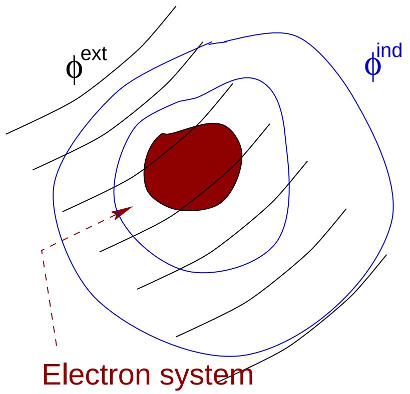
$$f_\Theta = \frac{2m^*}{\hbar}(\epsilon_\Theta - \epsilon_0)\left|(\Theta|\mathcal{H}^{rad}/\mathcal{E}^{ext}|0)\right|^2$$

Many-electron states



### HFA

Self-consistent linear response




$$\phi^{sc} = \phi^{ext} + \phi^{ind}$$

self-consistency: $\phi^{ind}$ depends on $\phi^{sc}$

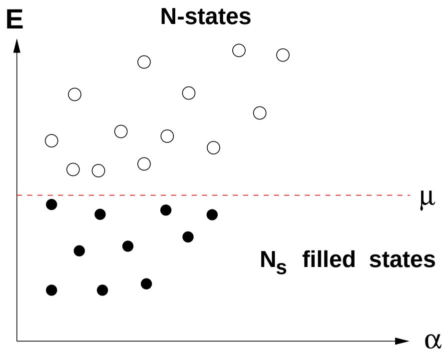
Vertex correction: $\phi^{ind} = \phi^{ind}_H + \phi^{ind}_{HF}$

Consistency → Kohn's theorem satisfied

THFA → later lecture

Empty states

$N > N_s$




Excitations

Collective modes $\leftrightarrow$ single-particle

Depolarization shift $\leftrightarrow$ interaction

Absorption $\leftrightarrow$ zeros of $\epsilon_{\alpha\beta}(\omega)$



DFT

Generally TLDA does not exist!

Kohn's theorem violated

Consistent theory built on current density

- G. Vignale and W. Kohn, Phys. Rev. Lett. **77**, 2037 (1996)

## Raman scattering

Inelastic light scattering → finite $\mathbf{q}$

No Kohn's theorem → relative modes

In resonance    off resonance

- Christoph Steinebach, submitted
- Single-particle excitations and many-particle interactions in quantum wires and dots, C. Schüller, G. Biese, K. Keller, C. Steinebach, D. Heitmann, P. Grambow, and K. Eberl Phys. Rev. B**54**, R17304-R17307 (1996)
- Spin-density and charge-density excitations in quantum wires, A. Brataas, A. G. Mal'shukov, C. Steinebach, V. Gudmundsson, K. A. Chao, Phys. Rev. B**55**, 13161 (1997)



## Tunneling

Models of open quantum dots

$\mu$ fixed by external potential

Coulomb blockade

### Correlation

Correlations between electrons cause suppression of most of energetically allowed tunneling processes involving excited dot states

cm.-modes are unaffected by correlation

Similarity with Kohn's theorem

- Selection rules for transport excitation spectroscopy of few-electron quantum dots, D. Pfannkuche and S. E. Ulloa, Phys. Rev. Lett. **74**, 1194 (1995)

## Type of interaction

- Screened Coulomb interaction
- $V \sim \frac{1}{r^2}$
- L. Quiroga, D. Ardila, and N. Johnson, Solid State Commun. **86**, 775 (1993)

Ideal model system to understand the Coulomb interaction