Interacting few body systems in magnetic fields

Tobias Kramer

Institut für Theoretische Physik, Universität Regensburg
and
Department of Physics, Harvard University

Cocoyoc, México, May 2012

Motivation: Hall effect

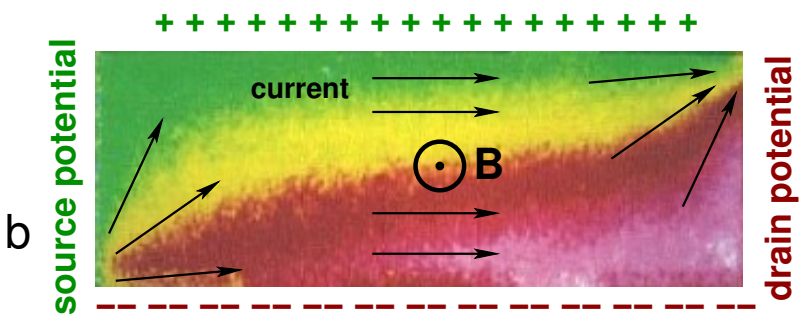
Edwin H. Hall:
Sometime during the last university year I was reading Maxwell's Electricity and Magnetism. (Maxwell: no permanent effect due to magnetism on current).
I brought the question to Prof. Rowland. He told me he doubted the truth of Maxwell's statement. I now began to give the matter more attention and ...

November 1879, experimental demonstration of the Hall effect.

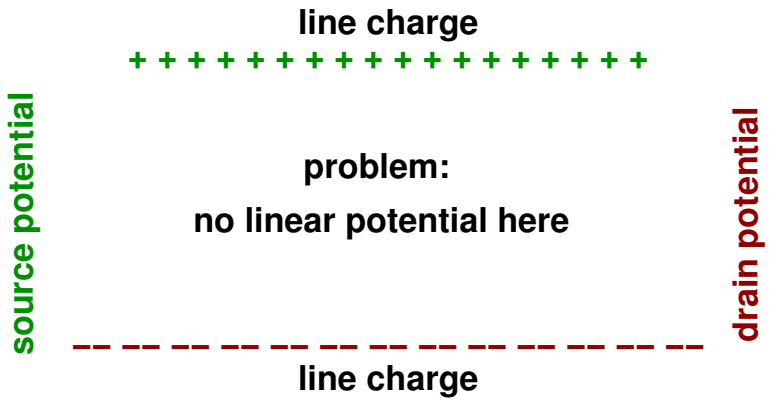
Theory?

Reminder: Hall effect

Textbook chapter: Sommerfeld theory of **non-interacting** electron gas.
Initially electrons get deflected, a charge builds up at the surface which generates a uniform electric field to exactly counter-balance the magnetic Lorentz-force.



Electric field measured to be uniform.
Experiment: Knott, von Klitzing (1995)



BUT: line charges not yield uniform field!

So where are the charges located in reality?
NO charge distribution in a plane yields uniform field!

Simple problem, no simple answer?!

From many to fewer electrons

Solving the many-body Schrödinger equation is a common theme across many fields. In this talk:

- what is the problem with the electrons in general and in magnetic fields?
- partial review of many-body approaches
- results ... and questions

Reduction: how to set us free from the curse of dimensionality

Solid-state device, operated in the quasi 2d-"quantum-regime" ($\boldsymbol{k_B T} < \hbar\boldsymbol{\omega_3}$), $\mathbf{10^2}$ — $\mathbf{10^6}$ electrons.

1. grid-based methods limited to small particle numbers or effectively non-interacting systems
2. density-funtional theory (DFT): reduce $\boldsymbol{N}$-particle wavefunction to a single density with only 3 coordinates!
   (misses important information: excitation energies? pair correlation function? still need to propagate Kohn-Sham system!)
3. classical dynamics: $\boldsymbol{N}$-particles described by trajectories $\{\vec{\boldsymbol{r}}_i(\boldsymbol{t}), \vec{\boldsymbol{v}}_i(\boldsymbol{t})\}$
4. coherent-state dynamics: TDSE written as set of "classical-like" equations of motions for an extended set of trajectories of variational parameters $\{\vec{\boldsymbol{r}}_i(\boldsymbol{t}), \vec{\boldsymbol{p}}_i(\boldsymbol{t}), \vec{\boldsymbol{w}}_i(\boldsymbol{t}), \ldots\}$

Alternative: mapping qm state to a classical (chaotic) system

Vandermonde polynomial $z_j = (x_j + \mathrm{i}y_j)$

$$f_{N+1}(z) = f_N(z) \prod_{j=1}^{N} (z_j - z_{N+1}) \tag{1}$$

Probability density:

$$|\psi(z_1, \ldots, z_N)|^2 = \prod_{j<k}^{N} |z_j - z_k|^2 \quad \mathrm{e}^{-\frac{1}{2}\sum_j^N |z_j|^2} \tag{2}$$

Laughlin: interpretation of probability density as a partition function of classical statistical mechanics

$$Z_{LLL} = \int \mathrm{dR}\ |\psi(z_1, \ldots, z_N)|^2 = \int \mathrm{dR}\ \mathrm{e}^{-\beta U_{\mathrm{cl}}(\mathrm{R})}, \tag{3}$$

$$U_{\mathrm{cl}}(\mathrm{R}) = -\sum_{j<k} \ln |z_j - z_k| + \frac{1}{4}\sum_j |z_j|^2 \tag{4}$$

$$\beta = 2 \tag{5}$$

Two kinds of interactions, #1: Pauli principle

Representation of the state by

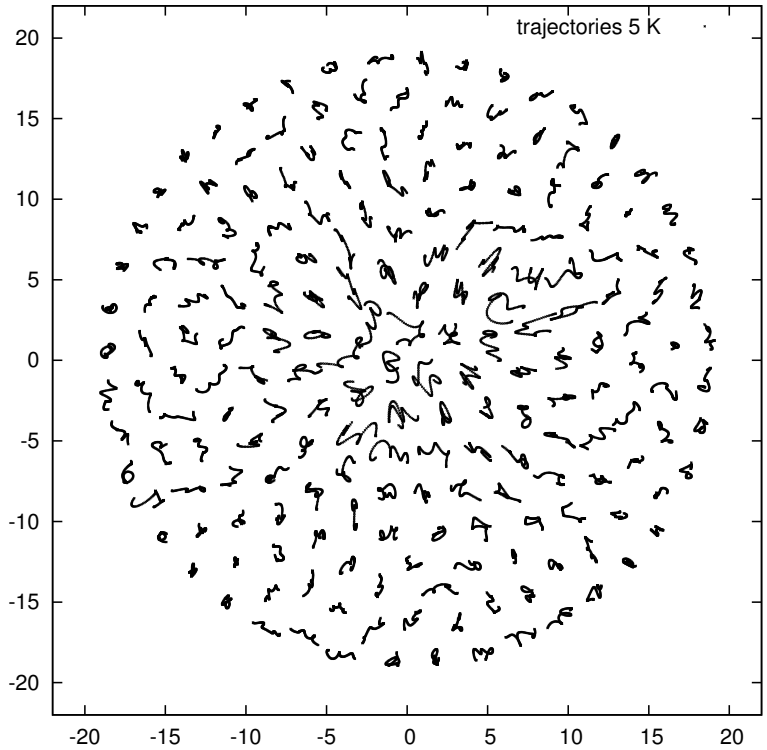
1. initially randomly chosen locations of classical electrons
2. let the electrons propagate with mutual logarithmic repulsion
3. check that the temperature is indeed equal to $\beta = 2$
4. sample for example the pair distribution function

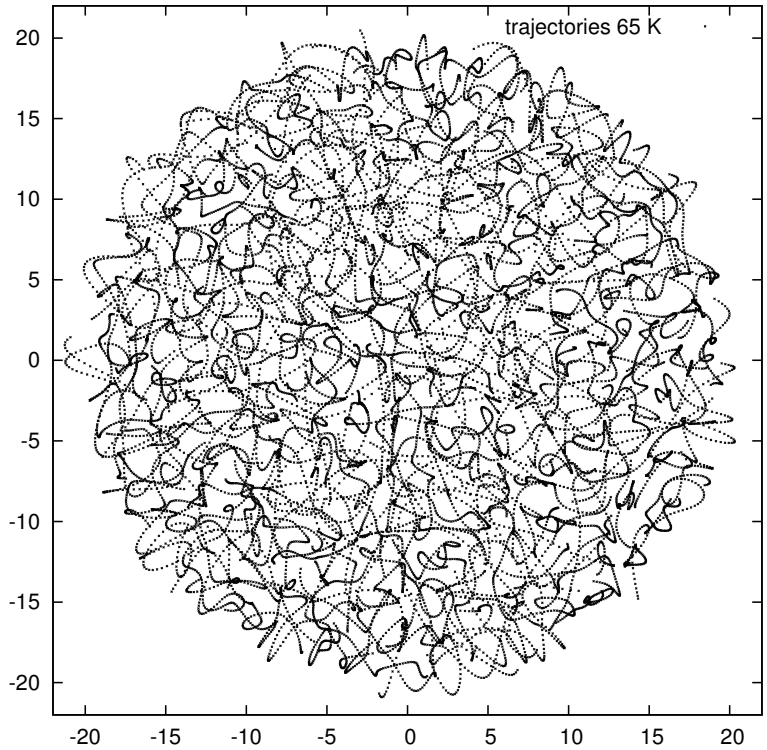
quantum mechanics:
$g_2(\mathbf{r}) = \int \mathrm{d}\mathbf{r}_2 \cdots \mathrm{d}\mathbf{r}_N |\psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2$

classical conditional probability:
if one of the particles is in a small volume around $(x + \Delta x, y + \Delta y)$,
where are the others?

Warm-up for electrons

196 electrons in a quantum-dot (logarithmic interaction, positive background)





Almost frozen configuration at $T = 5$ K

Thermal motion at $T = 65$ K

This procedure gives the Laughlin states and reproduces the Pauli-hole etc.

Conclusion: antisymmetrization is mapped to classical charges and dynamics at a specific temperature (for GaAs at 5 Tesla: Fermi-Dirac at $T = 0$ K mapped to Boltzmann at $T = 65$ K)

Two kinds of interactions, #2: Coulomb interaction

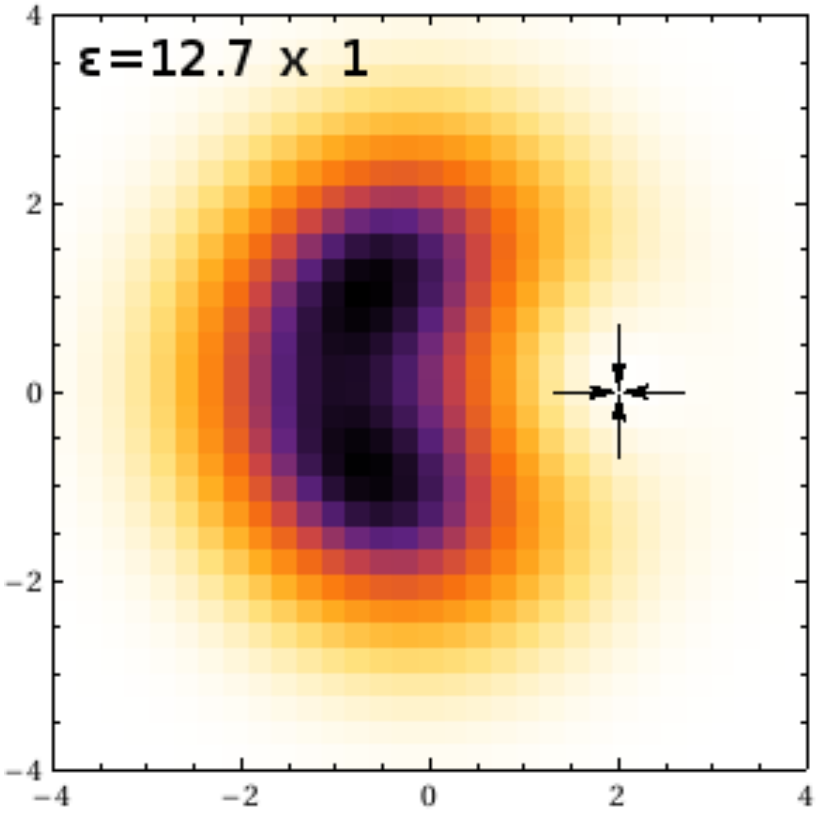
What happens if we add a “real force”, for example Coulomb force?
Representation of the new state by

1. initially randomly chosen locations of classical electrons
2. let the electrons propagate with mutual logarithmic and Coulomb repulsion
3. sample for example the pair distribution function

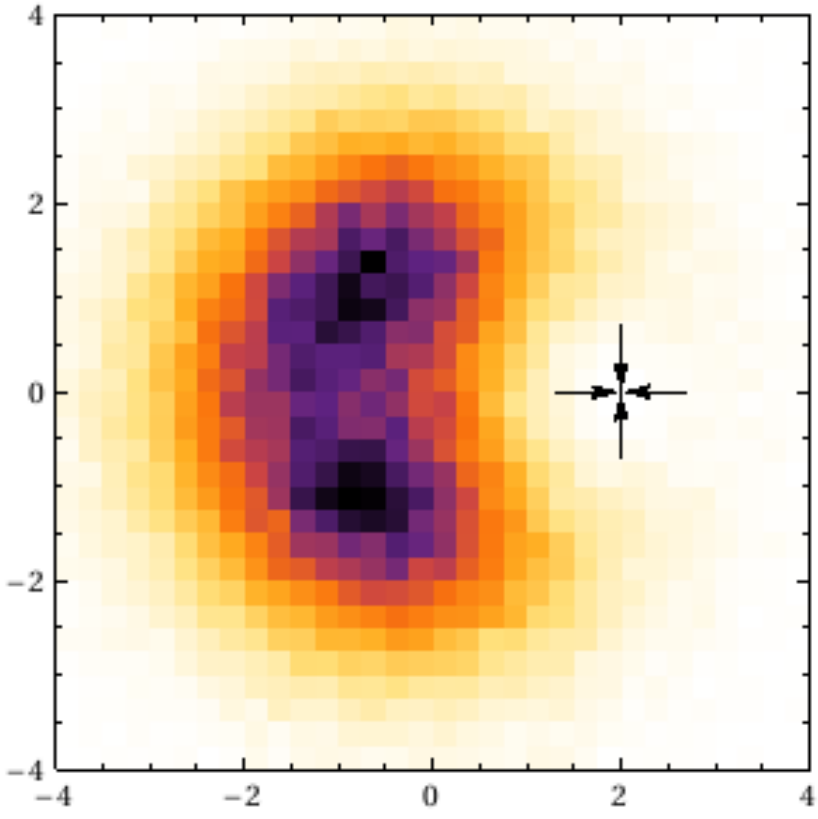
I compare the resulting pair distribution function to the QM result obtained by diagonalization of the interaction Hamiltonian.

Classical plasma with Pauli+Coulomb vs QM diagonalization

Example: three Coulomb interacting electrons in a magnetic field



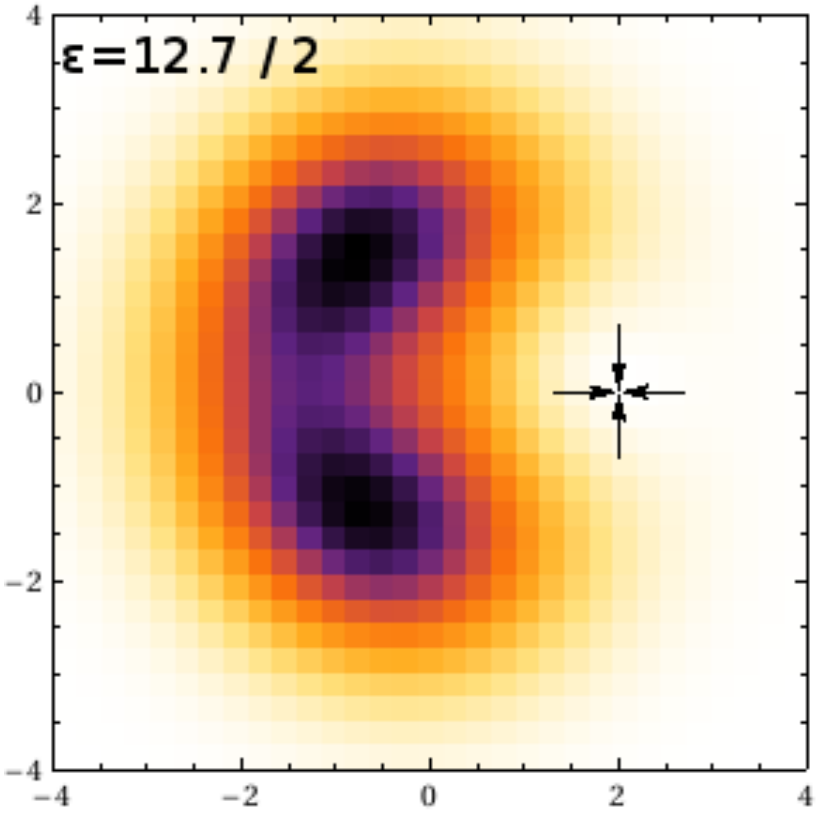
Pair distribution function via exact diagonalization



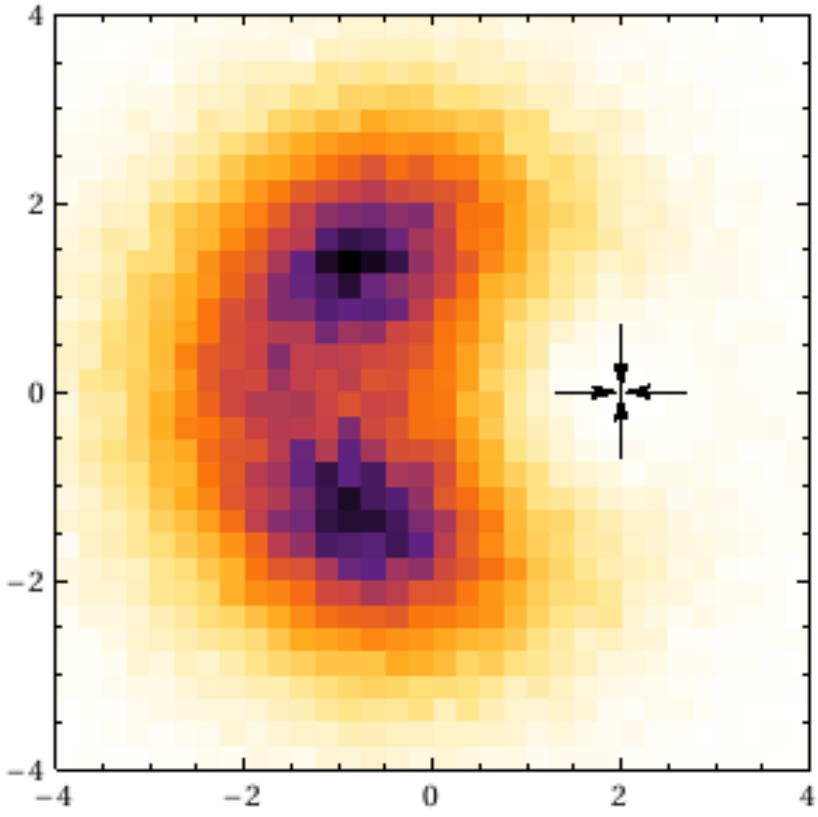
Pair distribution function from classical dynamics

Classical plasma with Pauli+Coulomb vs QM diagonalization

Example: three Coulomb interacting electrons in a magnetic field



Pair distribution function via exact diagonalization



Pair distribution function from classical dynamics

The time-dependent variational principle

Idea: put time-evolution in the parameters of a wave-packet and obtain equations of motions for the variational parameters. First rewrite TDSE

$$(\mathrm{i}\partial_t - H)\,|\psi\rangle = \frac{\langle\psi|\mathrm{i}\partial_t - H|\psi\rangle}{\langle\psi|\psi\rangle}|\psi\rangle, \quad |\phi\rangle = |\psi\rangle \exp\left[\mathrm{i}\int^t \mathrm{d}t' \frac{\langle\psi|\mathrm{i}\partial_t - H|\psi\rangle}{\langle\psi|\psi\rangle}\right]$$

Wave function parametrized by N complex variables $z(t)$ (coherent states!)

$$|\psi(t)\rangle = |\psi(z_1(t)\ldots z_N(t))\rangle, \quad N(z,\bar{z}) = \langle\psi(z)|\psi(z)\rangle, \quad \mathcal{H}(z,\bar{z}) = \frac{\langle\psi(z)|H|\psi(z)\rangle}{\langle\psi(z)|\psi(z)\rangle}$$

Equations of motion

$$C_{ij}(z,\bar{z}) = \frac{\partial^2}{\partial z_i \partial \bar{z}_j} \ln N(z,\bar{z}), \quad \mathrm{i}\begin{pmatrix} 0 & C \\ -\overline{C} & 0 \end{pmatrix}\begin{pmatrix} \dot{z} \\ \dot{\bar{z}} \end{pmatrix} = \begin{pmatrix} \partial_z \\ \partial_{\bar{z}} \end{pmatrix}\mathcal{H}$$

- E. Heller's work and articles on frozen/thawed Gaussians and wave packet dynamics.
- P. Kramer and M. Saraceno. Book: *The Geometry of the TDVP in QM*
- Y. Öhrn and E. Deumens. Review: *Dynamical, time-dependent view of molecular theory*
- H. Feldmeier and J. Schnack. Review: *Molecular dynamics for fermions*

Three interacting electrons in a quantum dot with magnetic field

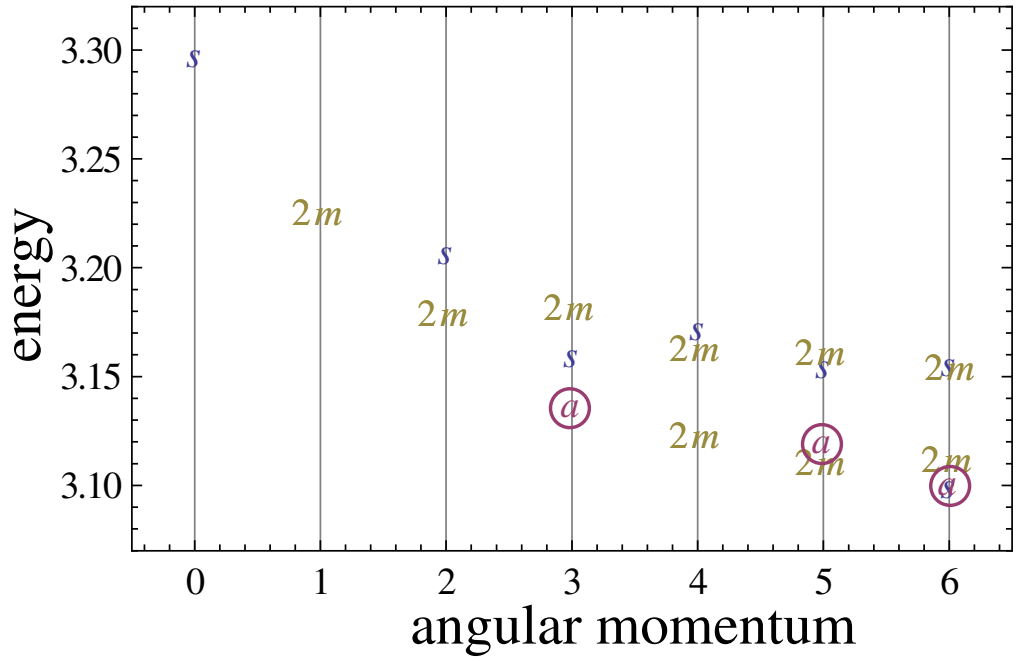
$$H = \sum_{i=1}^{N=3} \left[\frac{\mathbf{p}_i^{\,2}}{2m^*} + \frac{1}{2} m(\omega_0^2 + \omega_I^2)\mathbf{r}_i^2 - \omega_I L_{z,i} \right] + \sum_{i<j=1}^{N=3} \frac{e^2}{4\pi\epsilon_0\epsilon|\mathbf{r}_i - \mathbf{r}_j|}, \quad \omega_I = \frac{e\mathcal{B}}{2m}$$

Use TDVP to get trajectories $\{\vec{r}_i(t), \vec{p}_i(t)\} = \vec{z}(t)$, $i = 1, 2, 3$ for

$$\mathcal{H} = \frac{\langle\psi(\vec{z}(t))|H|\psi(\vec{z}(t))\rangle}{\langle\psi(\vec{z}(t))|\psi(\vec{z}(t))\rangle}, \quad \text{equations of motion} \frac{\partial\mathcal{H}}{\partial z} = \dot{z} \qquad (6)$$

The trajectory generates a (non-orthogonal) basis-set, use singular-value decomposition to obtain eigenstates and -energies.

Three-electron spectrum

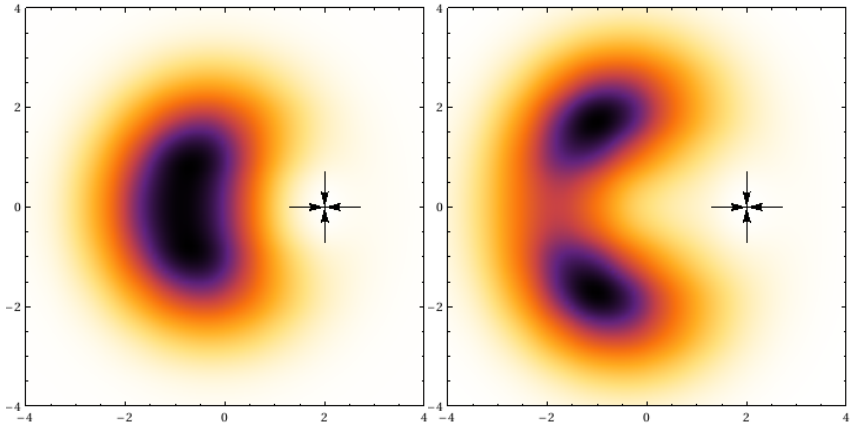


spatially **a**ntisymmetric, **s**ymmetric, **m**ixed symmetry

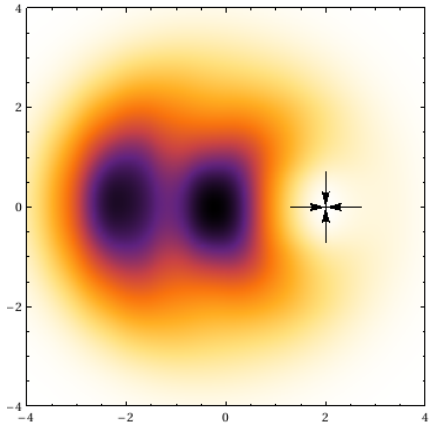
Essential point: do not include c.m.-motion! C.m. yields many shifted copies.
Classification: algebraic vibration-model (Iachello, Oss, Frank), (Moshinsky, P. Kramer)

Three-electron spectrum

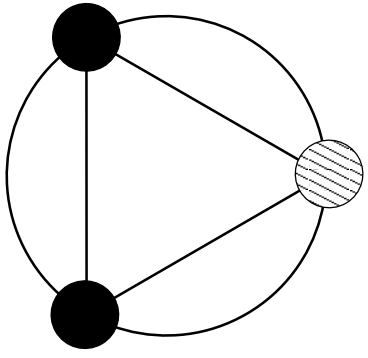
The pair-distribution function



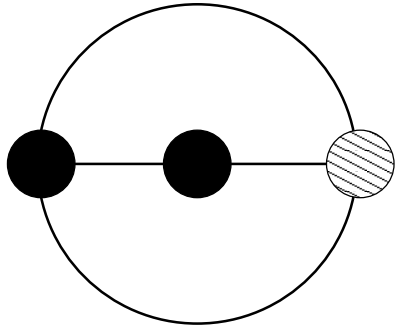
antisymmetric states with $L = 3, 6$



antisymmetric state with $L = 5$



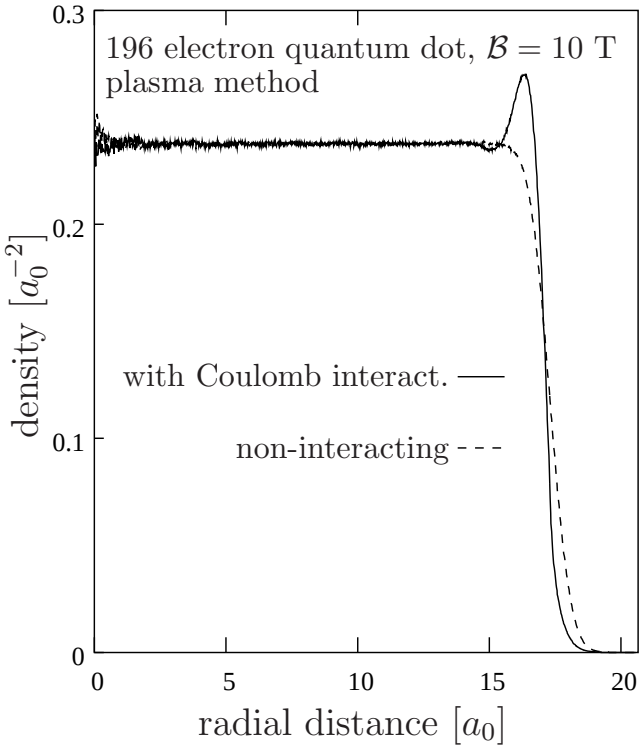
Lagrange

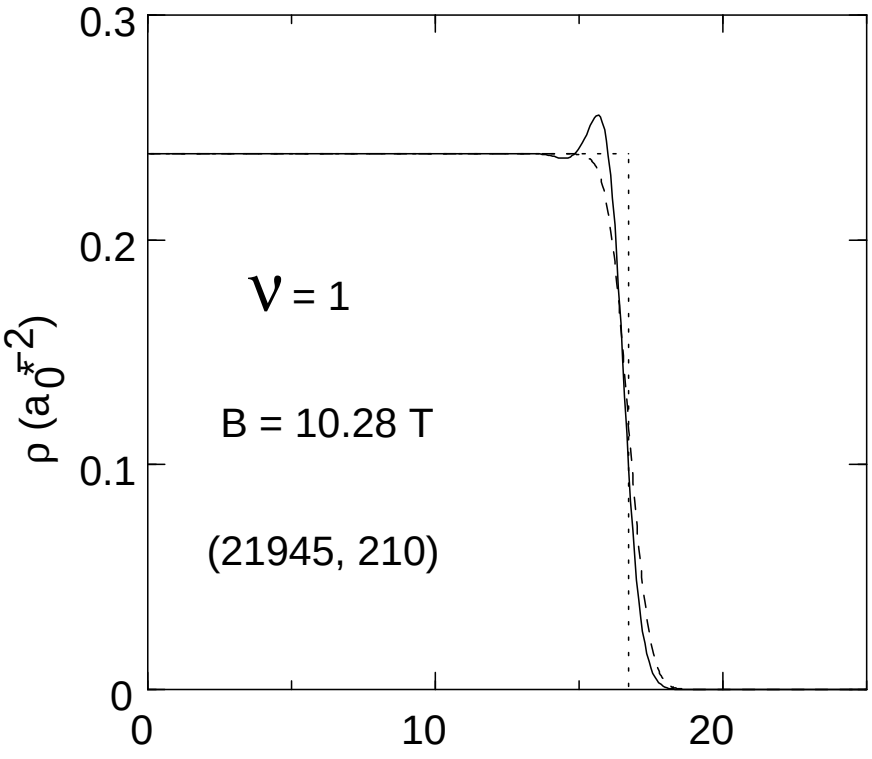


Euler

From 3 to 196 interacting electrons

Quantum dot with 196 e^-, magnetic field $\mathcal{B} = 10$ T, uniformly positive background.





Radial density profile
(classcial “ersatz dynamics”)
GPU calculation by TK (2012)

Radial density profile
(Current-Density-Functional-Theory)
Pi et al. PRB **57** 14783 (1998)

Summary

- The mapping of interacting qm many-body systems to a classical interacting system provides an interesting alternative to (TD)DFT (mapping to a non-interacting qm system).
- Both approaches need to map qm features of an electronic many-body wavefunction such as correct statistics. The classical map gives access to internal structure (pair distribution function)
- More work required to see if the maps works also for other configurations (also to compare with the “hypernetted-chain-approximation”, see M.W.C. Dharma-wardana *The classical-map hyper-netted-chain (CHNC) method and associated novel density-functional techniques for warm dense matter*, Internat. J. Quantum Chem. **112** p. 53 (2012))
- Insights from nuclear physics shed light on electronic structure calculations

References available at: www.quantumdynamics.de