Quantum coherence in many-body and few-body systems

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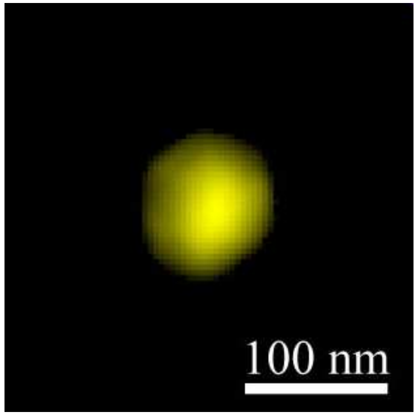
Introduction

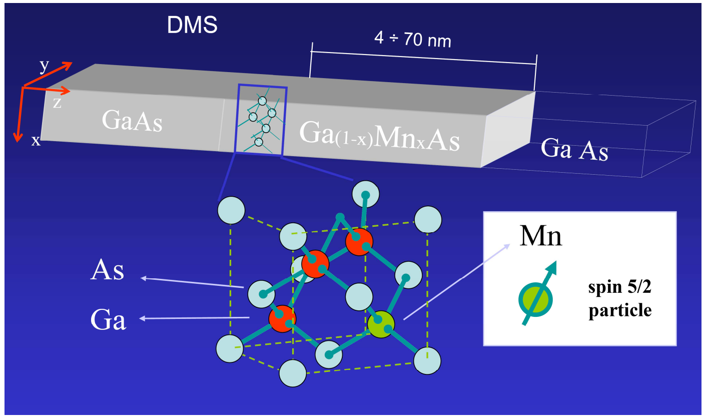
We are currently developing models to describe the electron (and spin) dynamics in…

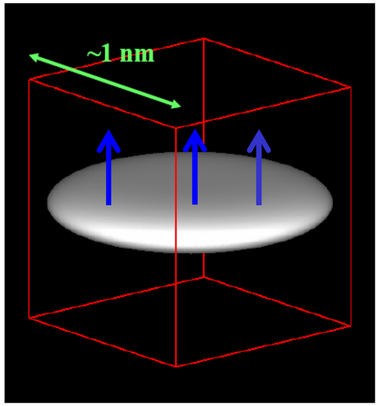
Metallic (alkali, noble) and semi-conductor (GaAs)

Nanostructures

Nanoparticles | Quantum Wells | Quantum Dots

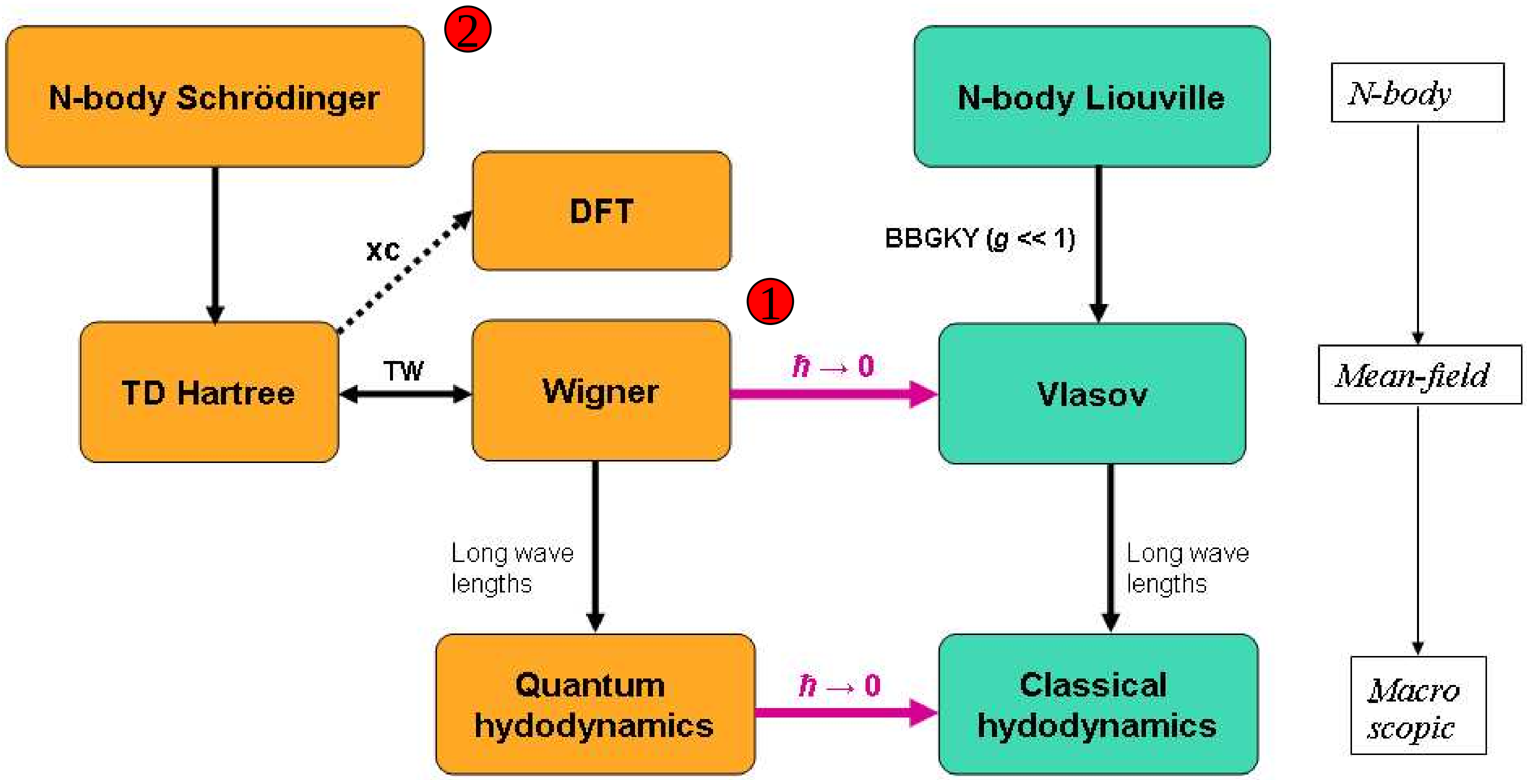






Dynamical models:hierarchy

quantum classical

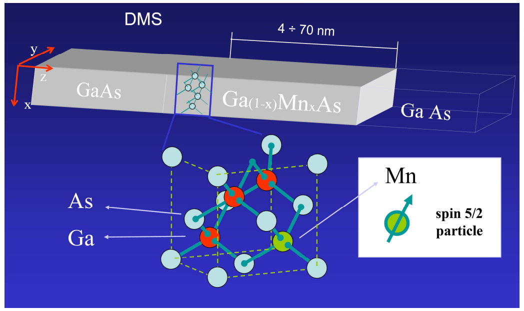


TW = Wigner transform

Outline

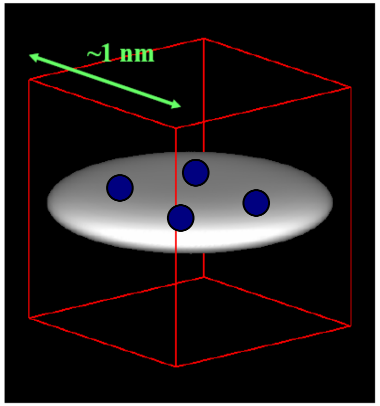
1) Many-body systems

Semiconductor quantum wells



Critical stability of quantum many-body systems <u>*in the time domain*</u>

2) Few-body systems ($N < 5$)



Quasi two-dimensional Gaussian quantum dot

Scales:

$l \sim$ nm

$n_e = 6\times10^{16}$ cm^{-3}

$T_e \sim 100$K

$\omega_0 = 10^{-12}$ s

Motivations (many-body)

• Small semiconductor devices are good candidates for possible applications in the emerging field of quantum computing

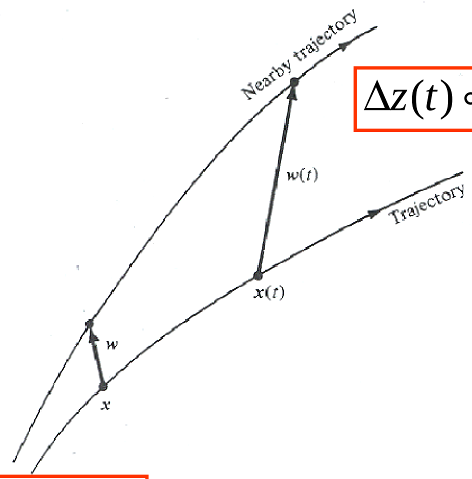
• To manipulate the electrons it is necessary to resort to electric fields, either static (dc) or oscillating (laser pulses)

• For many-electron devices it is therefore of paramount importance to understand the properties of the self consistent electron dynamics and its stability with respect to external perturbations

We want to characterize the stability of a quantum system against a small perturbation, simulating its "environment"

Dynamical stability: classical vs quantum

Classical



$$\boxed{\Delta z(t) \propto \exp(\lambda t)}$$

$$\boxed{\Delta z(t=0)}$$

λ = **Lyapunov** exponent

Quantum

- The Schrödinger equation is linear
- Initially close 'trajectories' will remain close
- No exponential separation

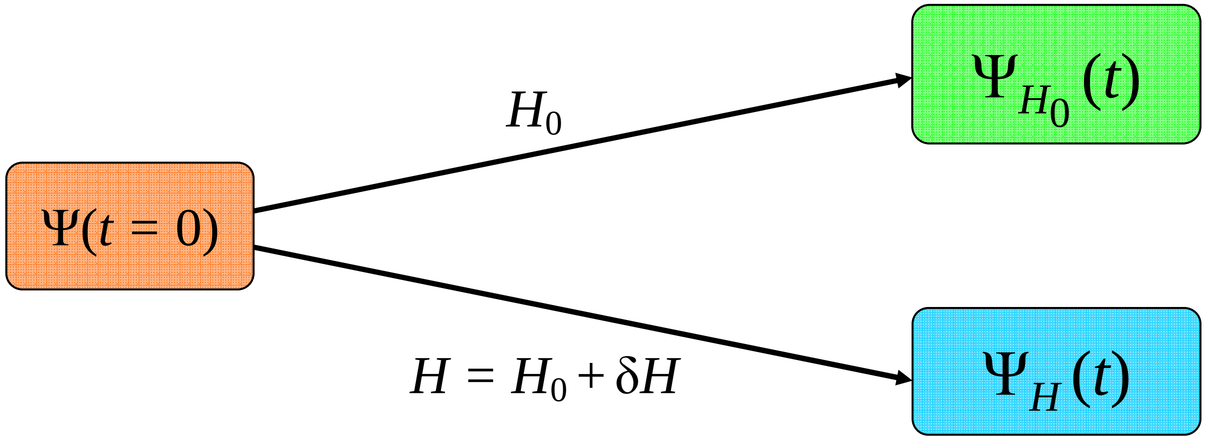
$$i\hbar \frac{\partial \psi_1}{\partial t} = H\psi_1$$

$$i\hbar \frac{\partial \psi_2}{\partial t} = H\psi_2$$

$$\frac{d}{dt}\langle \psi_2 | \psi_1 \rangle = 0$$

Quantum stability

- We want to characterize the stability of a quantum system against a small perturbation, simulating its “environment”.
- **A. Peres (1984): instead of perturbing the initial condition, perturb the Hamiltonian !**

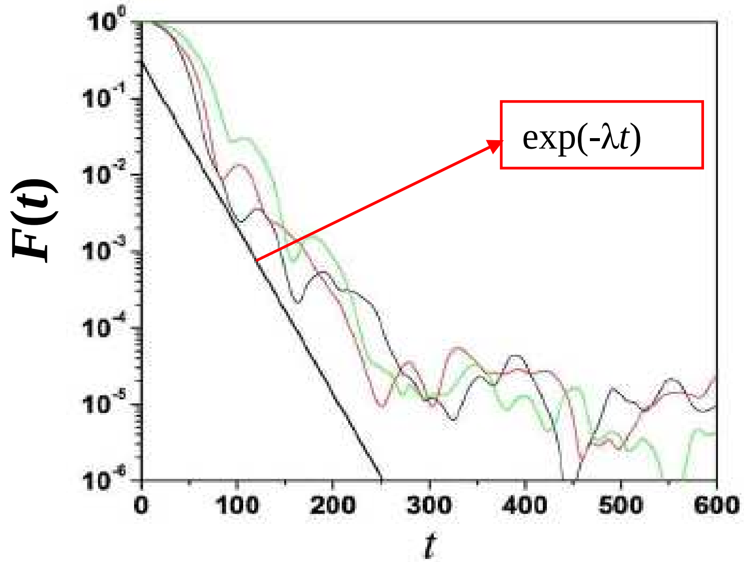


- Quantum stability is measured by the **quantum fidelity**

$$F(t) = \left|\langle \psi_{H_0}(t) | \psi_H(t) \rangle\right|^2.$$

Quantum fidelity for one-particle systems

- Single particle in a given (classically chaotic) Hamiltonian
- For medium-sized perturbations, the quantum fidelity decays exponentially, with a rate equal to the classical **Lyapunov** exponent
  - R. Jalabert and H. M. Pastawski, Phys. Rev. Lett. **86**, 2490 (2001)
- The rate is independent on the perturbation δH (universal behavior)



F. M. Cucchietti, H. M. Pastawski and D. A. Wisniacki, Phys. Rev. E **65**, 045206(R) (2002)

Review article: Ph. Jacquod and C. Petitjean (2009): Decoherence, entanglement and irreversibility in quantum dynamical systems with few degrees of freedom, Advances in Physics, **58**, 67-196 (2009)

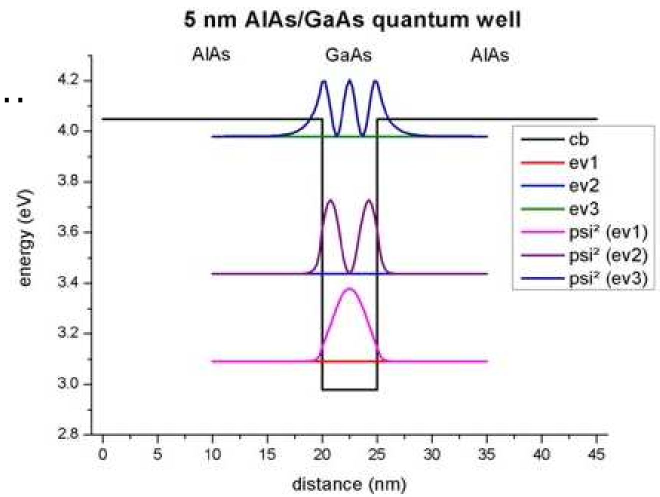
Many-particle systems

- All previous works focused on one-body dynamics in a given Hamiltonian
- What happens for the case of many interacting particles ?
- We have studied the quantum fidelity for **3** different many-body systems, all in the mean-field approximation
  - **System of interacting electrons:** Self-consistent set of quantum hydrodynamic equations [Phys. Rev. Lett. **97,** 190404 (2006)].
  - **Quantum wells**: Self-consistent Wigner–Poisson system [New J. Phys. **11**, 013050 (2009)].
  - **Trapped Bose-Einstein Condensate**: Gross-Pitaevskii equation (nonlinear Schrödinger equation) [Phys. Rev. Lett. 100, 050405 (2008)].

Coulomb interactions

Quantum wells: a paradigm for confined interacting electrons

- **Electron dynamics in finite-size systems**
  - **Semiconductor "quantum wells" and "quantum dots"**
  - Nanometric devices containing one or more electrons
  - Various types of confinement: parabolic, square well, …



Display a number interesting properties:

❖ **Finite size** *(due to confinement)*

❖ **Quantum** (*size of wave function ~ size of well*)

❖ **Collective** (*electrons interact*)

❖ **Nonlinear** (*strong excitations*)

Many-electron dynamics: a mean-field model

- **Wigner-Poisson equations** (single-band, effective-mass approximation)

$$\boxed{\begin{aligned}&\frac{\partial f}{\partial t}+v\frac{\partial f}{\partial x}+\frac{i m_*}{2\pi\hbar}\iint \mathrm{d}\lambda\,\mathrm{d}v' \mathrm{e}^{i m_*(v-v')\lambda} f(x,v',t)\\ &\times\left[V\left(x+\frac{\lambda\hbar}{2},t\right)-V\left(x-\frac{\lambda\hbar}{2},t\right)\right]=0\end{aligned}}$$

$f(x,v,t) =$ Wigner pseudo – probability distribution

- Total potential: $V = V_{\mathrm{H}} + V_{\mathrm{conf}}$

- Poisson equation for the Hartree potential: $\dfrac{\partial^2 V_{\mathrm{H}}}{\partial x^2} = \dfrac{e^2}{\varepsilon}\displaystyle\int_{-\infty}^{\infty} f\,\mathrm{d}v$

- Anharmonic confinement: $V_{\mathrm{conf}}(x) = \frac{1}{2}m_*\omega_0^2(x^2 + Kx^4).$ $\quad K << 1$

Dimensionless parameters

- **Normalized Planck constant**

$$\boxed{H = \hbar\omega_0/k_B T_e = \hbar/\sigma_x\sigma_p}$$

- **Ratio of electron plasma frequency to confinement frequency ("filling fraction"):**

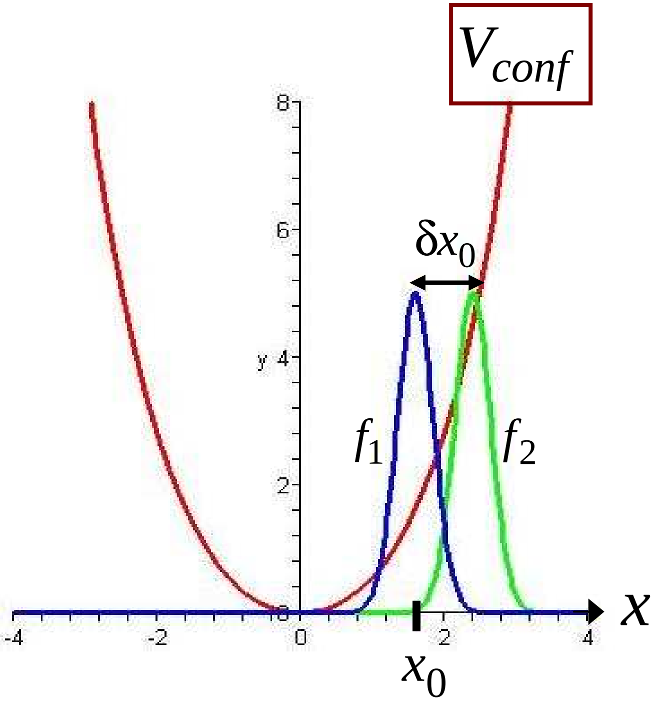
$$\boxed{\eta = \omega_p^2/\omega_0^2}$$

$$\omega_p = (e^2 n_e/m\varepsilon_0)^{1/2}$$

Time-evolution of the Wigner-Poisson system

Initial condition:

$$f_0(x,v) = \frac{n_e}{\sqrt{2\pi}\sigma_p} \exp\left(-\frac{(x-x_0)^2}{2\sigma_x^2} - \frac{{m_*}^2 v^2}{2\sigma_p^2} \right)$$

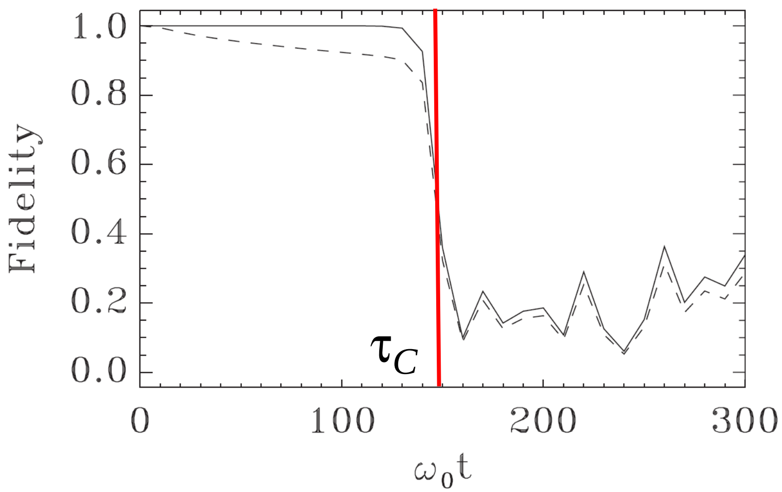


- We solve the Wigner Poisson equations for **two almost identical initial conditions**, which differ for a small initial perturbation.
- **Perturbation** : Small kick either in real space ($x \rightarrow x+\delta x_0$) or in velocity space ($\boldsymbol{v \rightarrow v+\delta v_0}$)
- Then compute the quantum fidelity:

$$F(t) = \frac{2\pi\hbar}{m_* N^2} \iint f_1(x,v,t) f_2(x,v,t)\, \mathrm{d}x\, \mathrm{d}v$$

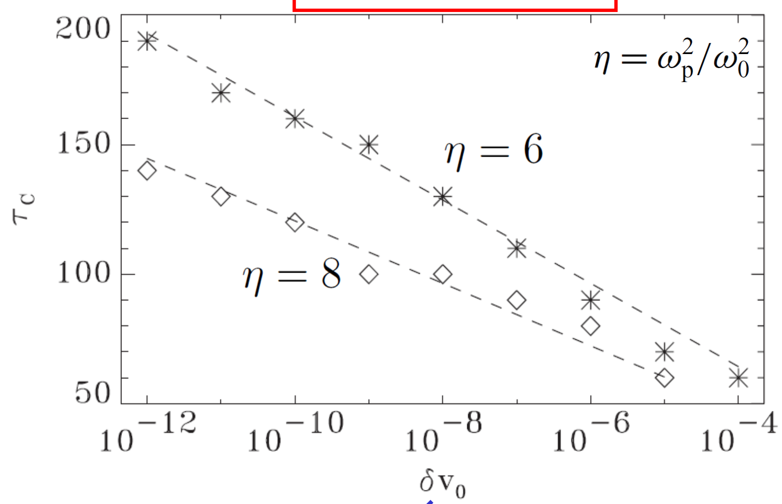
Quantum fidelity — results

$$F(t) = \frac{2\pi\hbar}{m_* N^2} \iint f_1(x, v, t)\, f_2(x, v, t)\, \mathrm{d}x\, \mathrm{d}v$$



$\eta = 6,\ H = 1,\ \delta v = 10^{-8} v_{\mathrm{th}}$

$\boxed{\tau_C = \text{critical time}}$



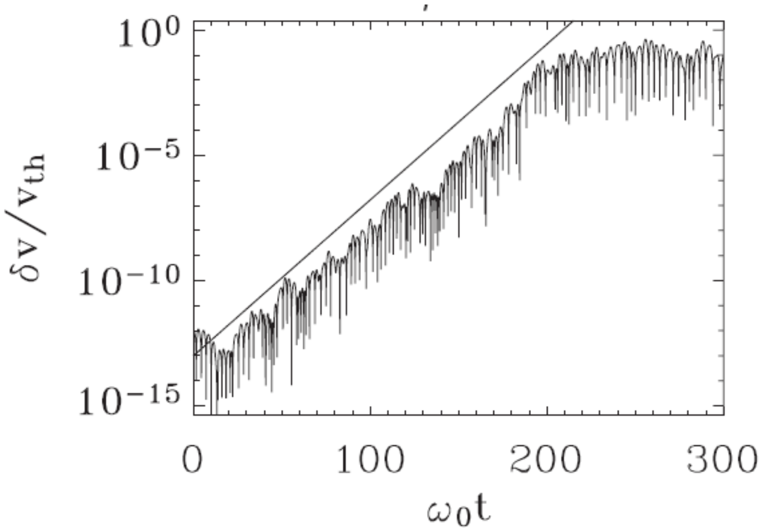
Initial perturbation

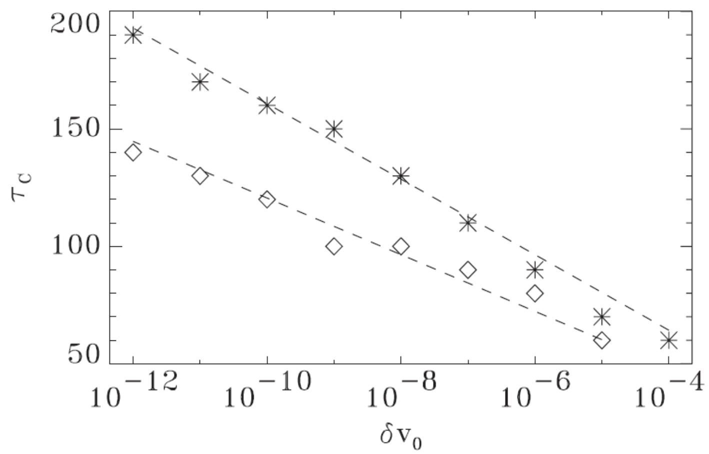
$$\tau_C = -\underset{?}{\underset{\uparrow}{\tau_0}} \ln \delta v_0 + \underset{?}{\underset{\uparrow}{\text{const.}}}$$

Trajectory separation

$$\langle v_i(t)\rangle = \iint f_i(x,v,t)\,v\,\mathrm{d}x\,\mathrm{d}v,\ i=1,2$$ Mean velocity

$$\delta v(t) = \langle v_1(t)\rangle - \langle v_2(t)\rangle \qquad \delta v(t=0)=\delta v_0.$$





$$\boxed{\delta v(t) = \delta v_0 \exp(\lambda t)}$$

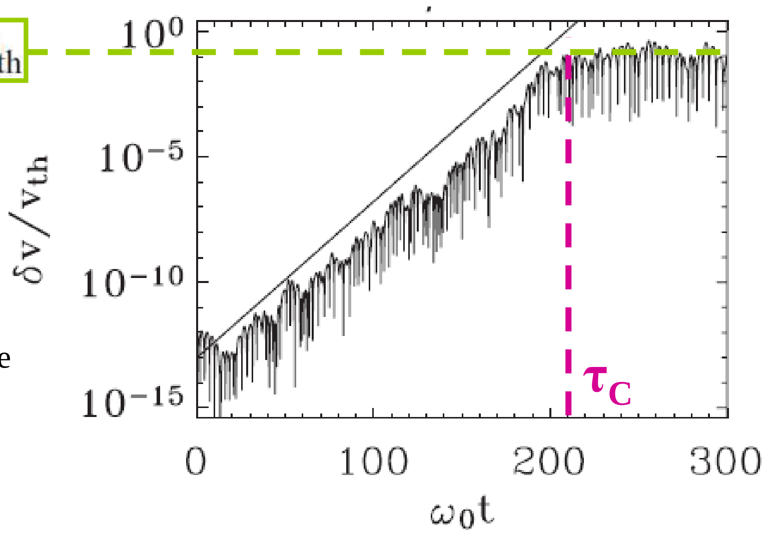
λ is a sort of "**Lyapunov** exponent"

$$\tau_C = -\tau_0 \ln \delta v_0 + \text{const.}$$

$$\boxed{\tau_0 = \frac{1}{\lambda}}$$

Trajectory separation and critical time

$$\boxed{\delta v_C \simeq \hbar/m_*\sigma_x = H v_{th}}$$



- **Conjecture:**

  The fidelity drop occurs when the trajectory separation reaches a critical value: $\delta v_C \simeq \hbar/m_*\sigma_x = H v_{th}$

critical value corresponds to a perturbation that is quantum-mechanically large

- This means that the initial perturbation has been amplified up to a magnitude comparable with **Planck**'s constant

- Then using $\delta v_C = \delta v_0 \exp(\lambda \tau_C)$ we get

$$\boxed{\tau_C = -\frac{1}{\lambda}\left[\ln\left(\frac{\delta v_0}{v_{th}}\right) - \ln H\right]}$$

Ehrenfest time

which correctly reproduces the numerical result (both the slope and the constant):

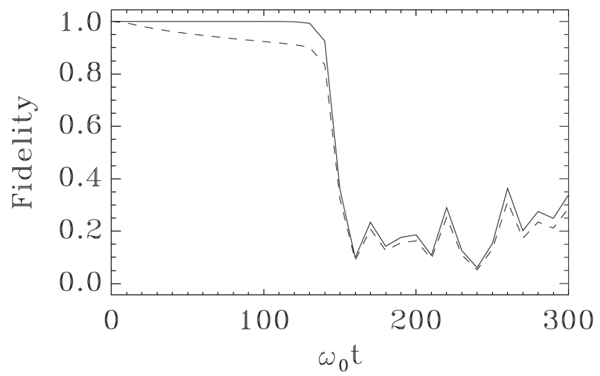
$$\boxed{\tau_C = -\tau_0 \ln \delta v_0 + \text{const.}}$$

Summary of key results

- **Critical time is linked to trajectory separation** (“**Lyapunov** exponent”)
  - The initial perturbation is amplified until it reaches a certain value (~ **Planck**’s constant)
  - Only then it starts affecting the fidelity

- **Sudden drop (instead of exponential decay) is a nonlinear effect**
  - When f_1 and f_2 start to diverge, also the Hamiltonian diverges (nonlinearity)
  - The Hamiltonian, in turns, acts on the evolutions of f_1 and f_2 , and so on
  - The outcome is a faster-than-exponential decay (“snowball effect”)

  - Instead, for the single-particle case, the Hamiltonian is fixed, and the evolutions diverge only because of the small perturbation. Hence, exponential decay



Effect of environmental decoherence (external)

- **Closed quantum systems (Hamiltonian)**
  - The evolution is **unitary**
  - Quantum coherence is measured by the **quantum fidelity**
  - Evolution of the wave function:
    - with a non-perturbed Hamiltonian: H_0
    - with a perturbed Hamiltonian: $H = H_0 + \delta H$

- **Open quantum systems (non-Hamiltonian: quantum Fokker-Planck)**
  - The evolution is **non-unitary**
  - **Decoherence** : deterioration of the "purity" of a quantum state via interaction to its environment.
  - Pure state ($t = 0$) $\rightarrow$ Mixed state ($t > 0$)

Effect of environmental decoherence (external)

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + \frac{im_*}{2\pi\hbar}\iint \mathrm{d}\lambda\, \mathrm{d}v' \mathrm{e}^{im_*(v-v')\lambda} f(x, v', t) \times \left[V\left(x + \frac{\lambda\hbar}{2}, t\right) - V\left(x - \frac{\lambda\hbar}{2}, t\right)\right] = \boxed{\left(\frac{\partial f}{\partial t}\right)_{\mathrm{scatt}}}$$

(à la **Zurek**)

$$\left(\frac{\partial f}{\partial t}\right)_{\mathrm{scatt}} = 2\gamma\frac{\partial(vf)}{\partial v} + D_v\frac{\partial^2 f}{\partial v^2} + D_x\frac{\partial^2 f}{\partial x^2}$$

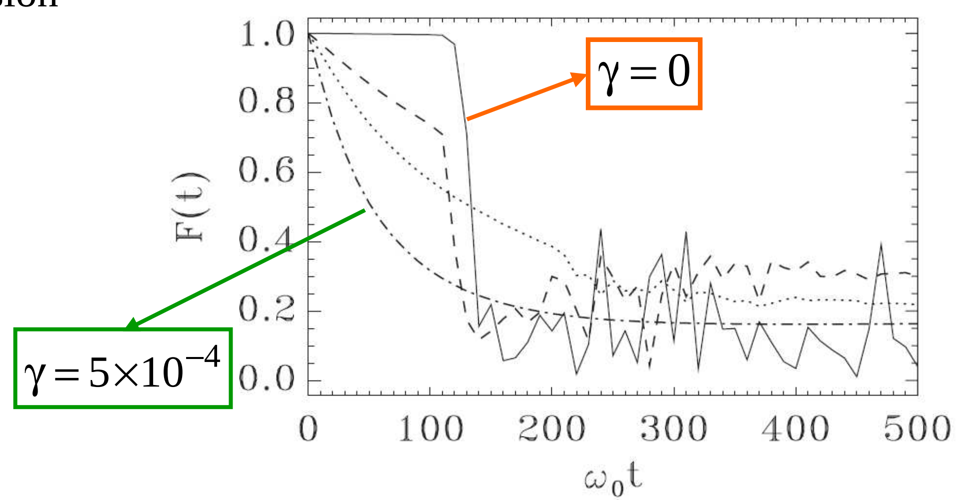
$$D_v D_x \geqslant \gamma^2\hbar^2/4m_*^2$$

$$D_v = \gamma v_{\mathrm{th}}^2$$

Lindblad form
(positivity of the density matrix)

γ: relaxation rate
D : diffusion

Quantum fidelity



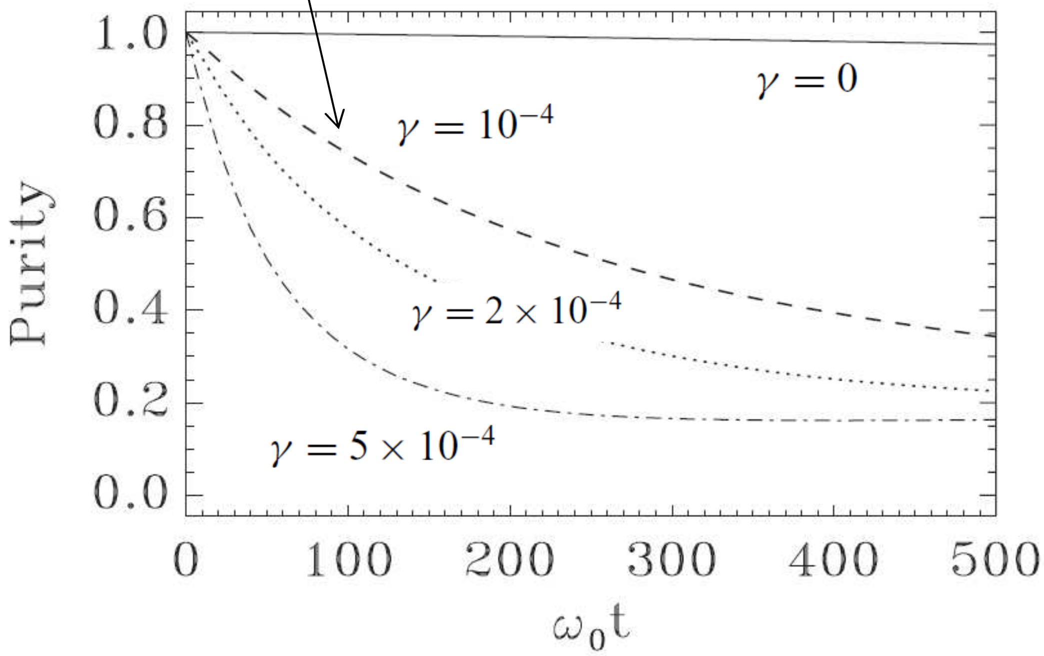
Effect of environmental decoherence (external)

Purity: $\boxed{\Sigma(t) = \frac{2\pi\hbar}{m_* N^2} \iint f^2 \,\mathrm{d}x\,\mathrm{d}v}$

$0 \leqslant \Sigma \leqslant 1$ for a mixed-quantum state

$\Sigma = 1$ for a pure state

decaying exponential



$\gamma/\omega_0 = 10^{-4}, 2 \times 10^{-4}$, and 5×10^{-4}

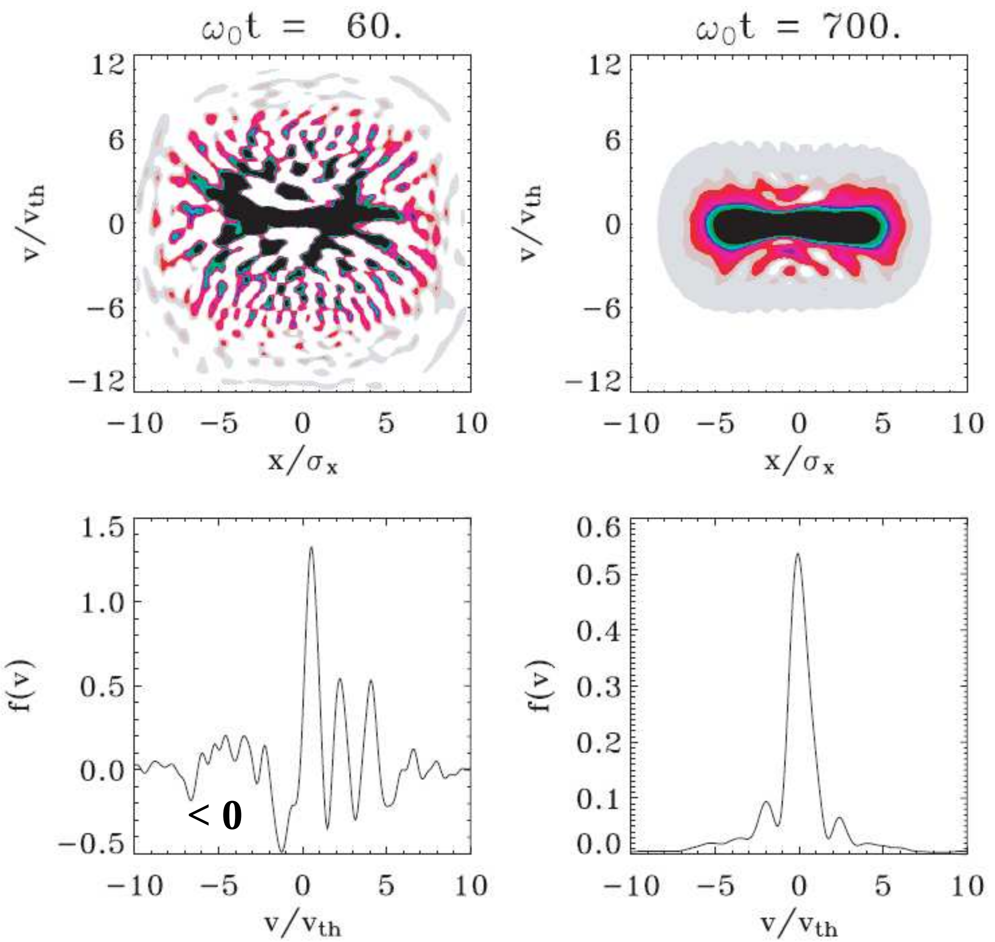
$\downarrow$

$\boxed{\omega_0 \tau_D = 234,\ 142 \text{ and } 58}$

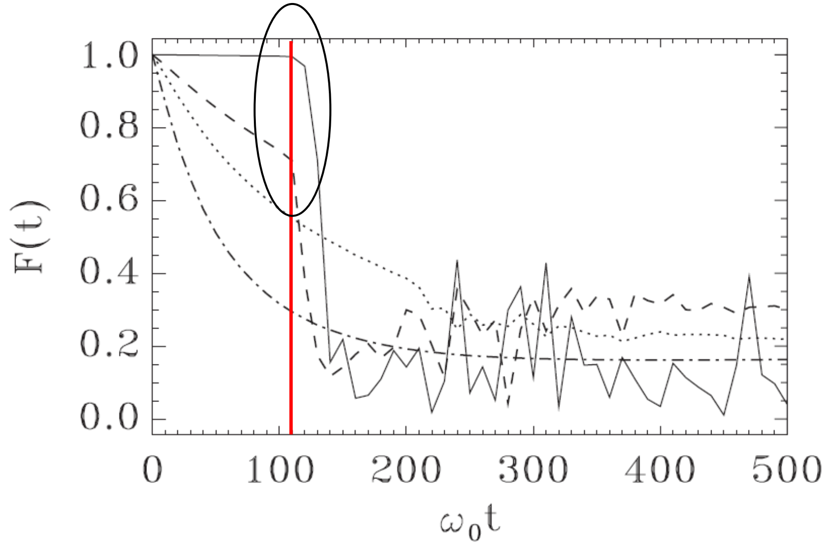
Phase-space portrait of the Wigner distribution (with dissipation)

Two gaussians centered at $x = \pm d/2$

$$\omega_0 \tau_D = 142$$



Decoherence



- First mechanism '**environment-induced decoherence**'
  - occurring on a timescale τ_D
  - dissipative
- Second '**internal decoherence**'
  - occurring on a timescale equal to τ_C
  - unitary (non-disipative)

Depending on the value of τ_D and τ_C, either mechanism will dominate in a specific situation

Conclusions

- **Stability of many-particle systems**
  - Unusual behavior of the quantum fidelity
  - Verified for 3 different types of modeling (all mean-field type)
    - Quantum hydrodynamics
    - Gross-Pitaevskii equation (NLSE)
    - Wigner-Poisson model

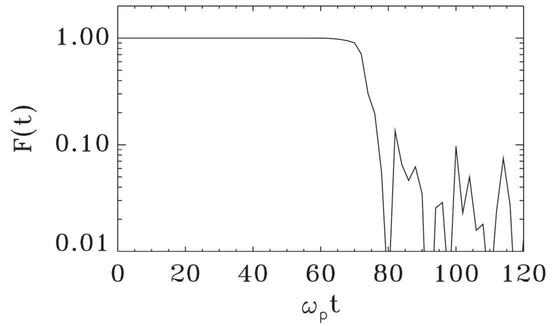
Is it typical of N-body interacting systems?

- **Perspectives**
  - Exact *N*-body problem
  - Under way: *N*=2 interacting electrons in a nonparabolic confinement

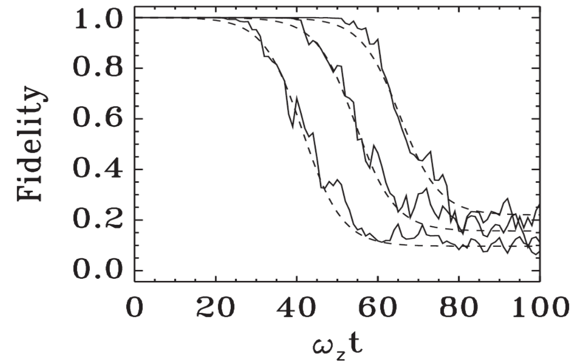
In collaboration with:
Sebastian Schröter and Javier Madronero
Physics Department, Technische Universität (München/Germany)

Quantum fidelity for other N-body system

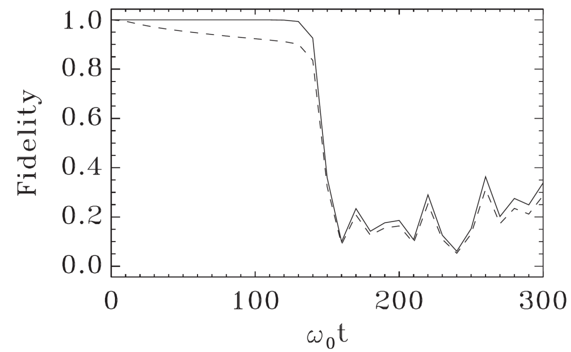
System of Interacting Electrons
Self-consistent set of quantum **hydrodynamic equations**
Periodic boundary conditions
Phys. Rev. Lett. **97,** 190404 (2006)



Trapped Bose-Einstein Condensate
Gross-Pitaevskii equation (nonlinear Schrödinger eq.)
Phys. Rev. Lett. **100,** 050405 (2008)



Quantum Wells
Self-consistent **Wigner–Poisson** system
New J. Phys. **11**, 013050 (2009)



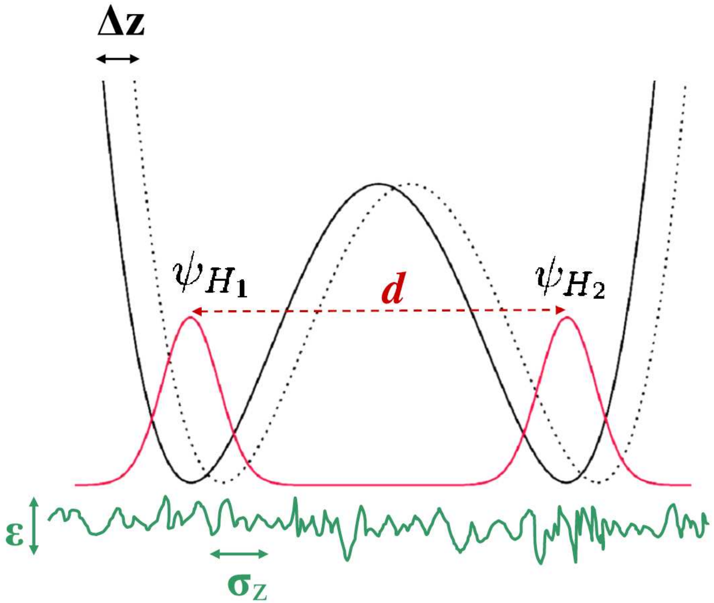
Quantum fidelity for other N-body system

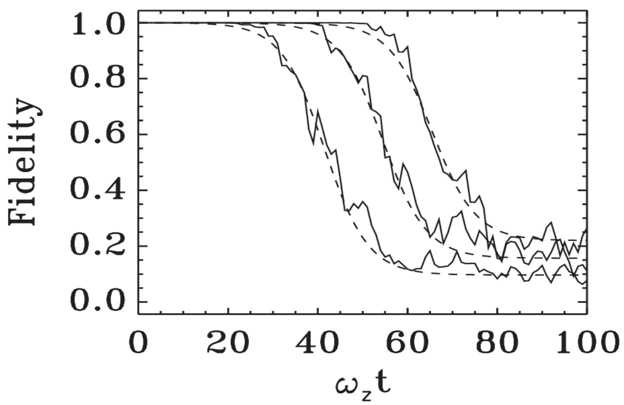
Trapped Bose-Einstein Condensate

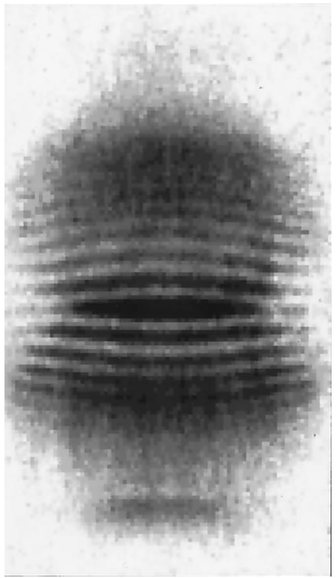
Gross-Pitaevskii equation (nonlinear Schrödinger eq.)

Phys. Rev. Lett. **100,** 050405 (2008)

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial z^2} + V(z)\psi + g_{1D}N_A|\psi|^2\psi \equiv H_0\psi$$





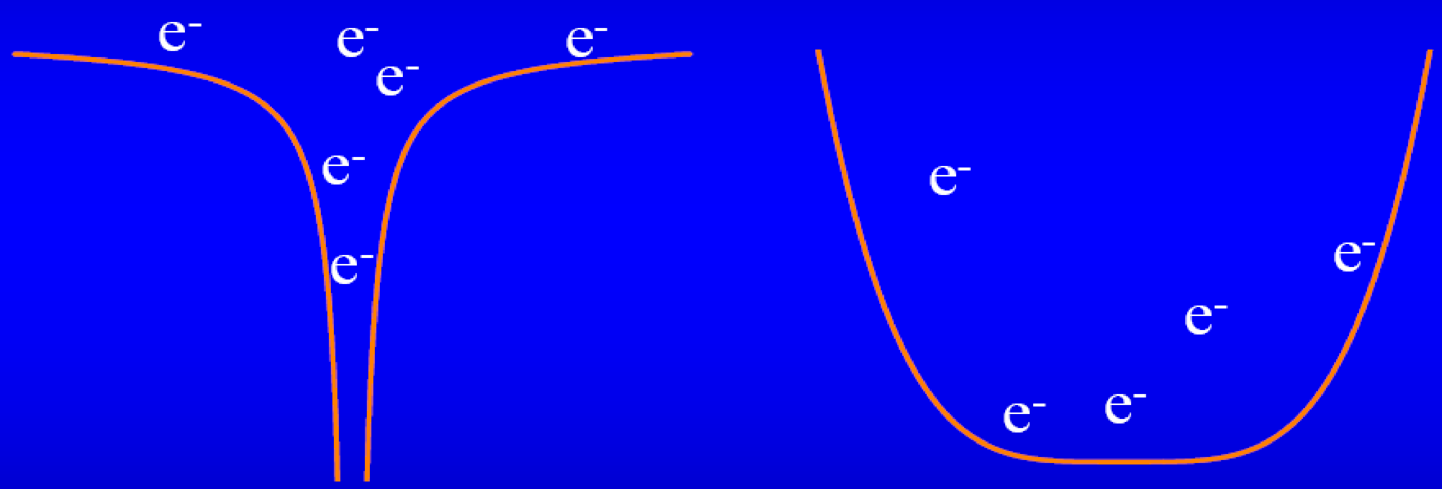


W. Ketterle et al (1997)

We predict that the contrast of the interference fringes will depend on the time t and on the perturbation ε, in a manner analogous to the quantum fidelity

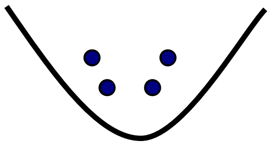
2) Few-body

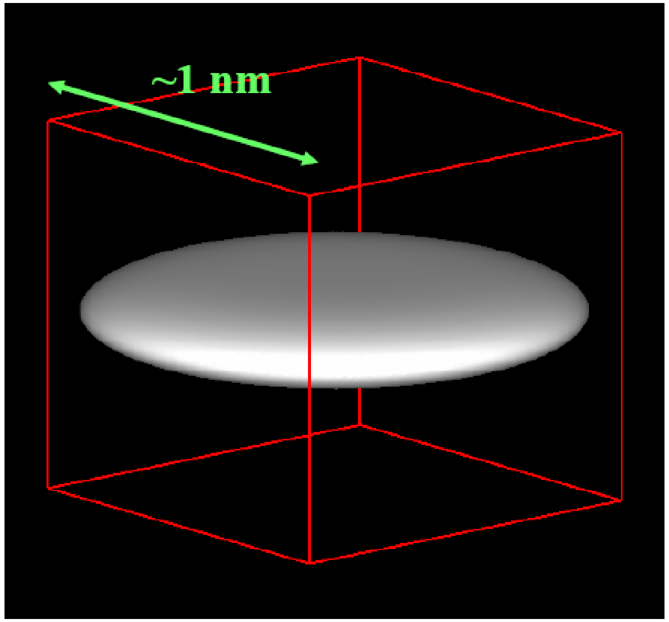
Many electron problems in non-Coulombic potential fields

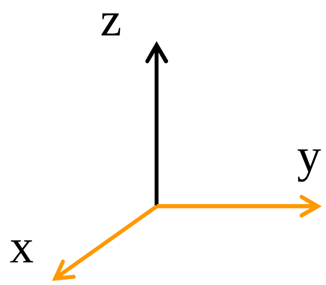


Coulomb	Non-Coulomb
Atomic φ	**Solid state φ**

Quasi two-dimensional Gaussian Quantum Dot



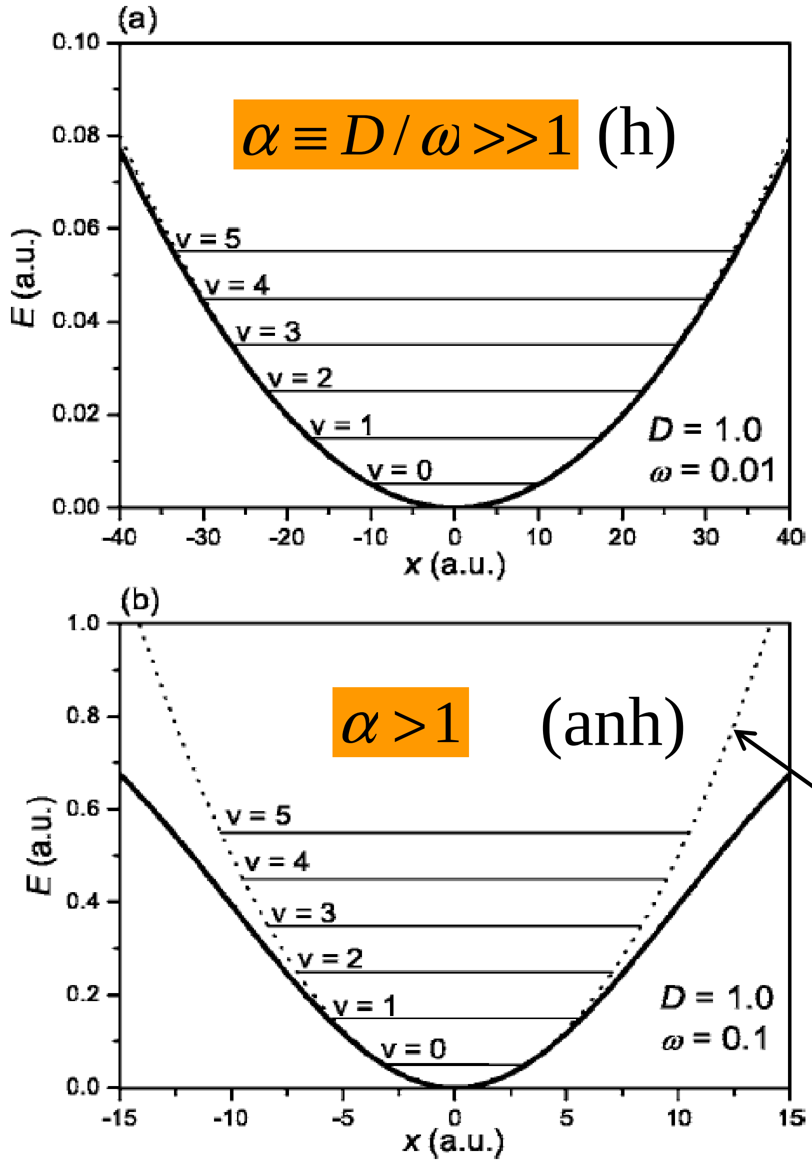




- → Gaussian confinement in 2 dimensions
- → Few electrons (2-4) are injected
- → One exactly solves the Schrödinger equation with **quantum chemistry methods** (CI) (post-Hartree)
- → One obtains the real wave-function of the excited states (/KS)

T. Sako, PAH and G. H. F. Diercksen, Phys. Rev. B **74**, 045329 (2006).

Quasi two-dimensional Gaussian Quantum Dot



$$[\mathcal{H}(\boldsymbol{r}) + \mathcal{W}(\boldsymbol{r})]\Psi(1,2,\ldots,N) = E\Psi(1,2,\ldots,N)$$

$$\mathcal{H}(\boldsymbol{r}) = \sum_{i=1}^{N}\left[-\tfrac{1}{2}\nabla_i^2\right] + \sum_{i>j}^{N}\left[\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}\right]$$

$$\mathcal{W}(\boldsymbol{r}) = \sum_{i=1}^{N} w(\boldsymbol{r}_i)$$

Multi-electronic Hamiltonian

$$w(\boldsymbol{r}_i) = -D\exp[-\gamma(x_i^2 + y_i^2)] + \frac{1}{2}\omega_z^2 z_i^2$$

$$\omega = \sqrt{2D\gamma}$$

Gaussian confinement

Harmonic potential

CI method

Few words about CI…

→ Natural set of basis functions is the Hartree-Fock basis set φ_i^{HF}

$$\left.\begin{aligned} H\varphi_i^H &= -\frac{\hbar^2}{2m}\frac{\partial^2\varphi_i^H}{\partial x^2} - e\phi\varphi_i^H \\ \frac{\partial^2\phi}{\partial x^2} &= \frac{e}{\varepsilon_0}\left(\sum_{i=1}^N \left|\varphi_i^H\right|^2 - n_i\right) \end{aligned}\right\} \text{Hartree equations}$$

Poisson equation

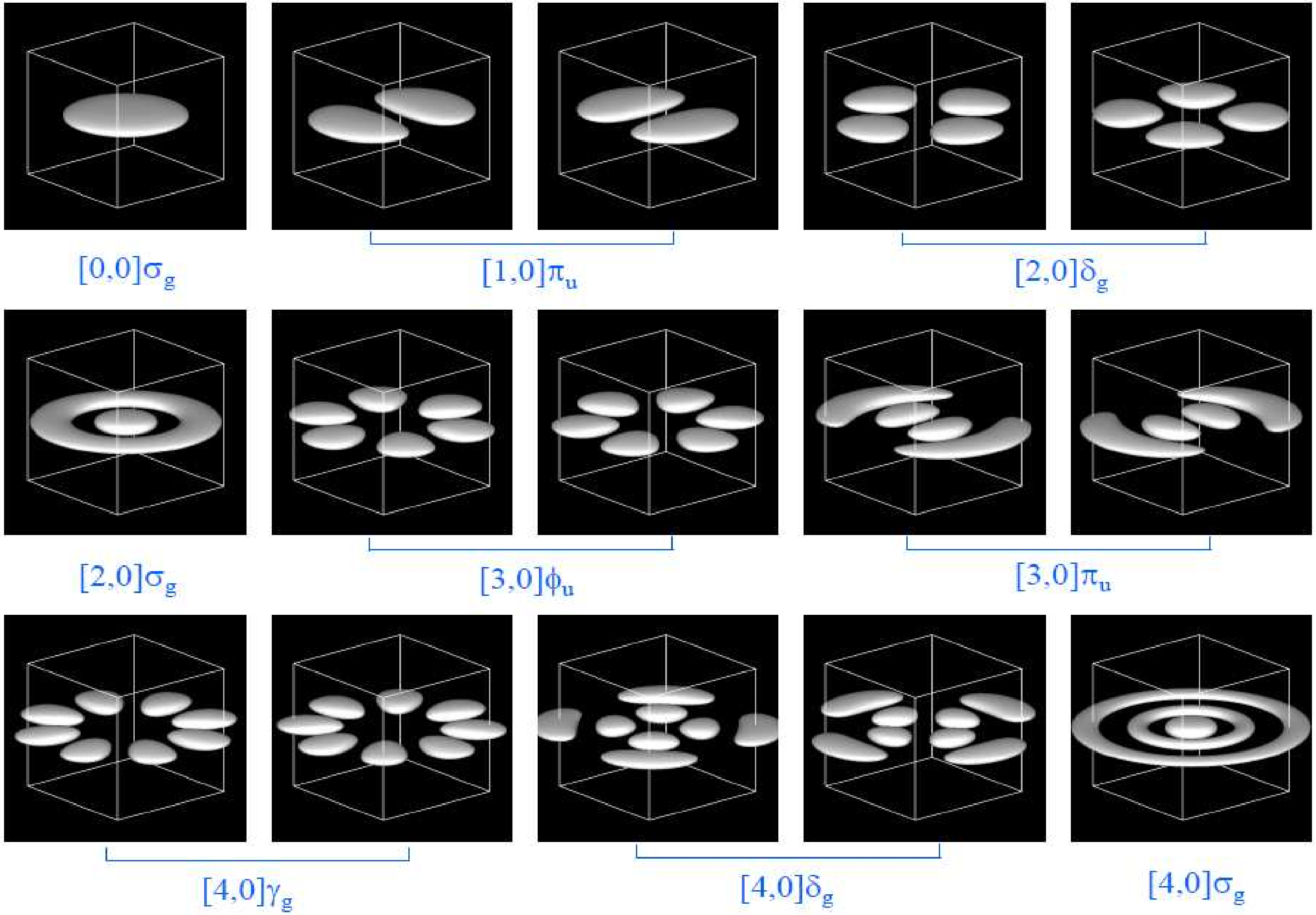
→ We add the Pauli principle → Slater determinants

CI $\longrightarrow$ $\boxed{\psi = \sum_k a_k \varphi_k^{HF}}$ $\longrightarrow$ $\boxed{\min\langle\psi|H|\psi\rangle}$

→ The choice of the configuration is an art…especially for the molecular case (Tokuei Sako / Tokyo) **(Open-Mol/gaussians)**

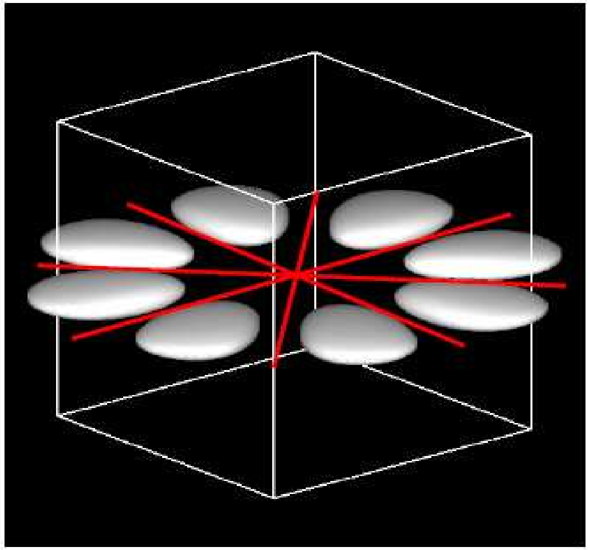
Quantum Dots

Hartree-Fock orbitals



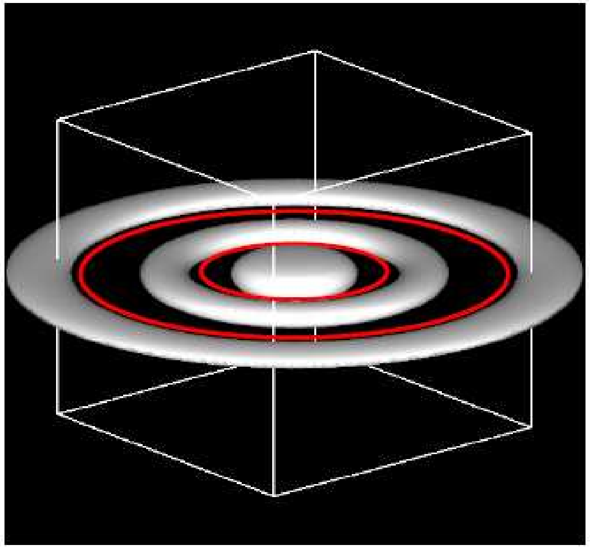
Quantum Dots

Two-types of electron modes



Circular mode

$$|l_z| = 4$$

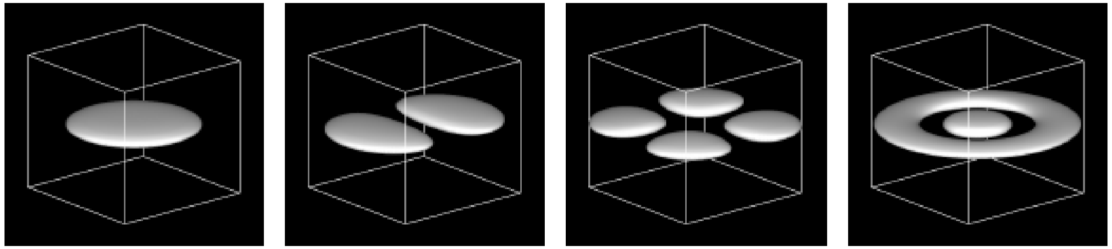


Breathing mode

$$n = 4$$

Polyad quantum number v_p

$$3^5\Pi_u \quad : \quad ([0,0]\sigma_g)([1,0]\pi_u)([2,0]\delta_g)([2,0]\sigma_g)$$



$$v_p = \quad 0 \quad + \quad 1 \quad + \quad 2 \quad + \quad 2 \quad = 5$$

W. Low, Phys. Rev. **97**, 1664 (1955).

G. D. Saksena, J. Chem. Phys. **31**, 839 (1959).

Quantum Dots

Leading configurations

	State	Configuration	Weight	v_P
$2e$	$^{*}1\,{}^1\Sigma_g^+$	$([0,0]\sigma_g)^2$	0.84	0
	$1\,{}^1\Pi_u$	$([0,0]\sigma_g)([1,0]\pi_u)$	0.76	1
	$2\,{}^1\Pi_u$	$([1,0]\pi_u)([2,0]\sigma_g)$	0.31	3
	$3\,{}^1\Pi_u$	$([0,0]\sigma_g)([3,0]\pi_u)$	0.54	3
	$^{*}1\,{}^3\Pi_u$	$([0,0]\sigma_g)([1,0]\pi_u)$	0.86	1
	$1\,{}^3\Sigma_g^+$	$([0,0]\sigma_g)([2,0]\sigma_g)$	0.80	2
	$1\,{}^3\Delta_g$	$([0,0]\sigma_g)([2,0]\delta_g)$	0.82	2
	$1\,{}^3\Sigma_g^-$	$([1,0]\pi_u)([1,0]\pi_u)$	0.77	2
	$2\,{}^3\Delta_g$	$([0,0]\sigma_g)([4,0]\delta_g)$	0.28	4
$3e$	$^{*}1\,{}^2\Pi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)$	0.70	1
	$1\,{}^2\Sigma_g^+$	$([0,0]\sigma_g)^2([2,0]\sigma_g)$	0.43	2
	$2\,{}^2\Sigma_g^+$	$([0,0]\sigma_g)([1,0]\pi_u)^2$	0.37	2
	$2\,{}^2\Delta_g$	$([0,0]\sigma_g)^2([2,0]\delta_g)$	0.43	2
	$1\,{}^2\Sigma_g^-$	$([0,0]\sigma_g)([1,0]\pi_u)([1,0]\pi_u)$	0.63	2
	$2\,{}^2\Sigma_g^-$	$([0,0]\sigma_g)([2,0]\delta_g)([2,0]\delta_g)$	0.16	4
	$3\,{}^2\Delta_g$	$([0,0]\sigma_g)([2,0]\delta_g)([2,0]\sigma_g)$	0.22	4
	$3\,{}^2\Sigma_g^+$	$([0,0]\sigma_g)([2,0]\sigma_g)^2$	0.26	4
	$3\,{}^2\Sigma_g^-$	$([0,0]\sigma_g)([1,0]\pi_u)([3,0]\pi_u)$	0.44	4
	$^{*}1\,{}^4\Sigma_g^-$	$([0,0]\sigma_g)([1,0]\pi_u)([1,0]\pi_u)$	0.88	2
	$1\,{}^4\Pi_u$	$([0,0]\sigma_g)([1,0]\pi_u)([2,0]\sigma_g)$	0.85	3
	$2\,{}^4\Pi_u$	$([0,0]\sigma_g)([1,0]\pi_u)([2,0]\delta_g)$	0.84	3
	$3\,{}^4\Pi_u$	$([0,0]\sigma_g)([1,0]\pi_u)([4,0]\delta_g)$	0.33	5
$4e$	$^{*}1\,{}^1\Delta_g$	$([0,0]\sigma_g)^2([1,0]\pi_u)^2$	0.56	2
	$1\,{}^1\Pi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)([2,0]\delta_g)$	0.34	3
	$2\,{}^1\Pi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)([2,0]\sigma_g)$	0.32	3
	$1\,{}^1\Phi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)([2,0]\delta_g)$	0.50	3
	$3\,{}^1\Pi_u$	$([0,0]\sigma_g)([1,0]\pi_u)^2([1,0]\pi_u)$	0.21	3
	$3\,{}^1\Phi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)([4,0]\gamma_g)$	0.23	5
	$5\,{}^1\Pi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)([4,0]\sigma_g)$	0.15	5
	$4\,{}^1\Phi_u$	$([1,0]\pi_u)([1,0]\pi_u)^2([2,0]\delta_g)$	0.16	5
	$^{*}1\,{}^3\Sigma_g^-$	$([0,0]\sigma_g)^2([1,0]\pi_u)([1,0]\pi_u)$	0.62	2
	$2\,{}^3\Pi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)([2,0]\sigma_g)$	0.45	3
	$3\,{}^3\Pi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)([2,0]\delta_g)$	0.29	3
	$4\,{}^3\Pi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)([1,0]\pi_u)([3,0]\pi_u)$	0.12	5
	$5\,{}^3\Pi_u$	$([0,0]\sigma_g)^2([1,0]\pi_u)([2,0]\delta_g)([2,0]\delta_g)$	0.11	5
	$^{*}1\,{}^5\Delta_g$	$([0,0]\sigma_g)([1,0]\pi_u)([1,0]\pi_u)([2,0]\delta_g)$	0.87	4
	$1\,{}^5\Phi_u$	$([0,0]\sigma_g)([1,0]\pi_u)([2,0]\delta_g)([2,0]\sigma_g)$	0.38	5
	$1\,{}^5\Pi_u$	$([0,0]\sigma_g)([1,0]\pi_u)([1,0]\pi_u)([3,0]\pi_u)$	0.59	5
	$2\,{}^5\Phi_u$	$([0,0]\sigma_g)([1,0]\pi_u)([1,0]\pi_u)([3,0]\phi_u)$	0.59	5
	$2\,{}^5\Pi_u$	$([0,0]\sigma_g)([1,0]\pi_u)([2,0]\delta_g)([2,0]\delta_g)$	0.69	5
	$3\,{}^5\Pi_u$	$([0,0]\sigma_g)([1,0]\pi_u)([2,0]\delta_g)([2,0]\sigma_g)$	0.38	5

Quantum Dots

Dipolar transitions (laser such that $\lambda >> d$)

Long wave-length approximation

a → b $$f_{ba} = 2(E_b - E_a)\left|\left\langle \psi_b \left| \sum_{i=1}^{N_e} z_i \right| \psi_a \right\rangle\right|^2$$ Oscillator strengths

One should verify

$\sum_b f_{ba} = N_e$ TRK sum rule

Kohn's theorem:

Phys. Rev. **123**, 1242 (1961).

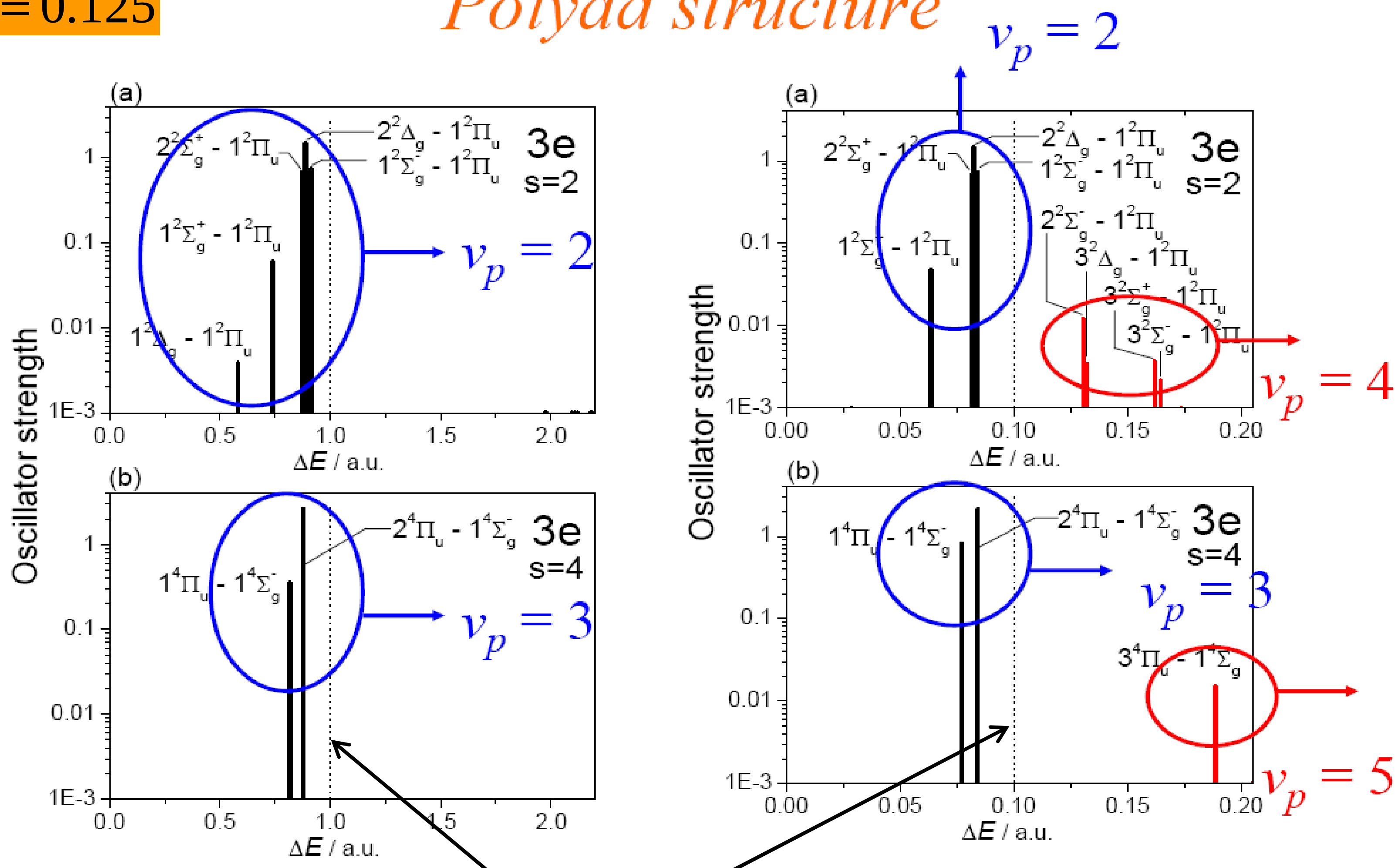
For an external harmonic potential, the motion of the center-of-mass is completely decoupled from the one of the internal degrees of freedom [$\forall$ the shape of v($\mathbf{r}_1$-$\mathbf{r}_2$)]

Comment: this is true only for an exact treatment of the *N*-body problem !

Quantum Dots (3 electrons)

$\alpha = 0.125$

Polyad structure

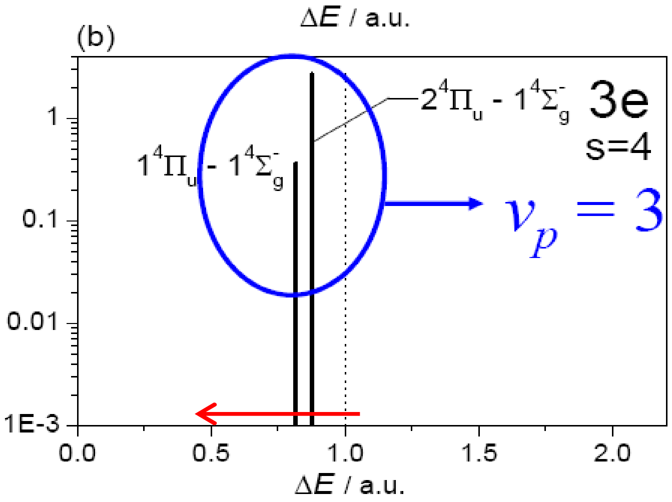


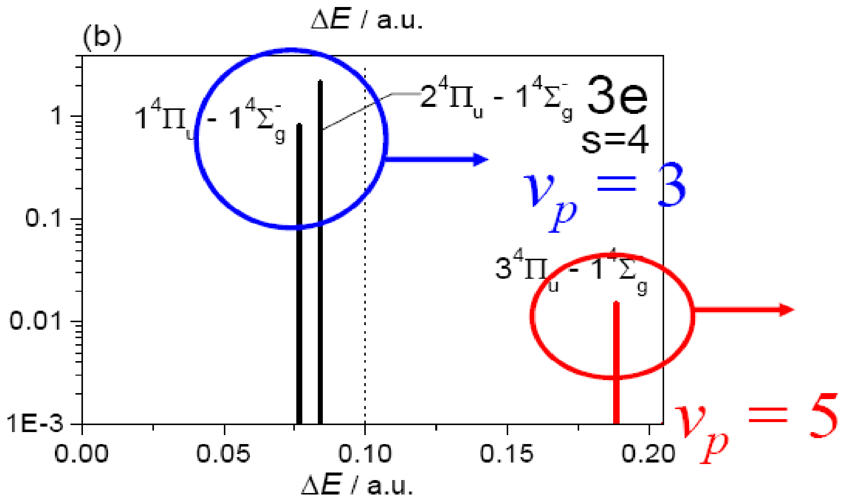
Kohn

smaller e-e / conf. $\omega = 1.0$

$\omega = 0.1$ **larger e-e / conf.**

Quantum Dots (3 electrons)





smaller e-e / conf. ω = 1.0

ω = 0.1 **larger e-e / conf.**

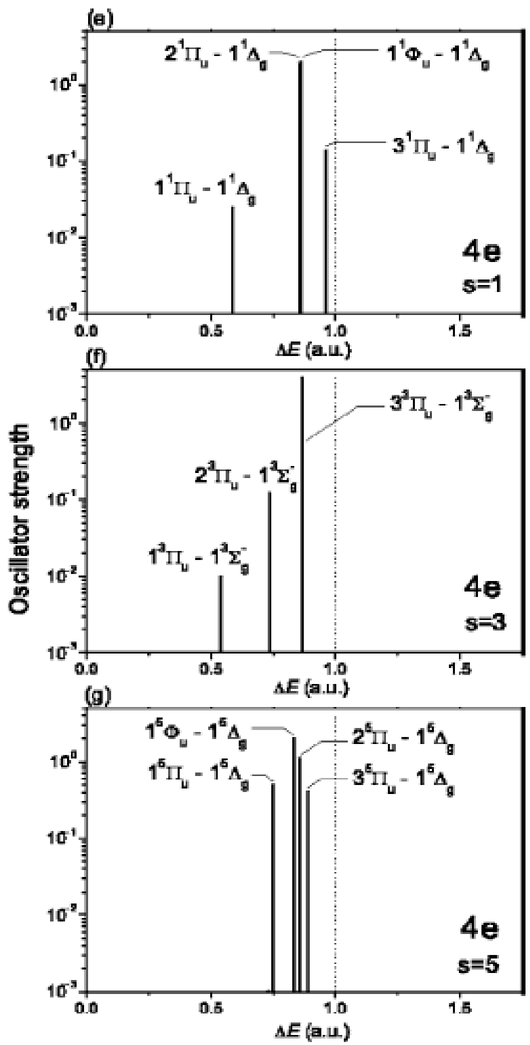
→ Red shift of the **Kohn** mode with the anharmonicities

→ For **large ω**: transitions only at low energy + transitions of states having the same « polyad » numbers: those of the center-of-mass

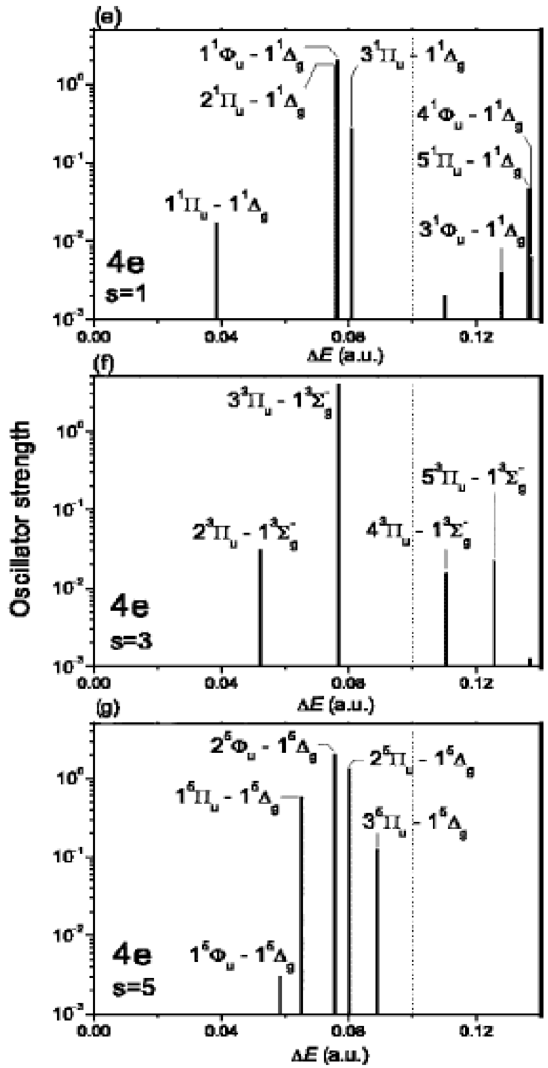
→ For **small ω**: transitions at low and high energy + transitions of states having the same « polyad » numbers or differing by 2 from the *com.*

The **e-e** interactions **are stronger in this case**.

Quantum Dots (4 electrons)



large ω



small ω

Messages

→ In order to include decoherence processes (interaction with an enviroment) in the quantum dynamics: **Wigner**

The existence of a finite internal decoherence suggests that even in the absence of coupling to an external environment a many-body quantum system might not, in practice, be perfectly reversible !

→ The methods of **quantum chemistry** can be successfully applied to the modelling of few-body nanostructures