

Excitation of radial collective modes in a quantum dot: Beyond linear response

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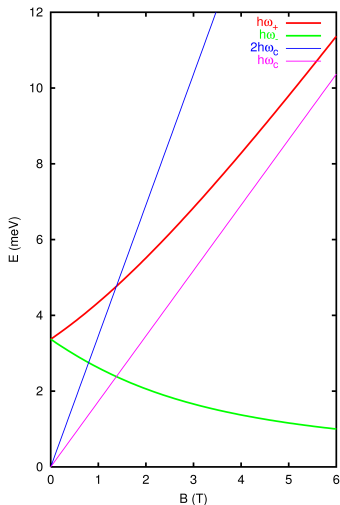
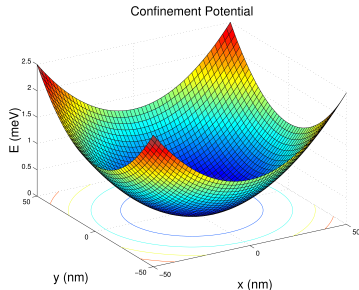
Annalen der Physik **526**, 235 (2014), DOI:10.1002/andp.201400048
<http://arxiv.org/abs/1311.3252>

- What about exact time-evolution in a system with fixed number of electrons?
- External energy pumped in for a short time
- Nonlinear response?
- What is nonlinear? – Comparison to mean-field models

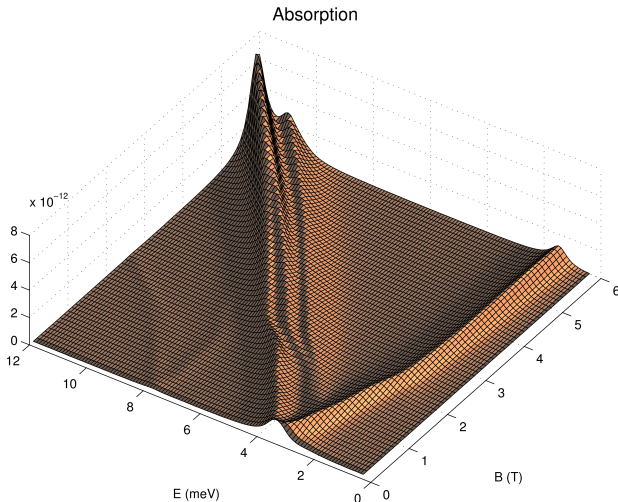
Kohn's theorem

- Exact
- FIR-radiation, dipole
- Parabolic confinement

→ Only stiff CM-motion



Calculated power absorption, **soft confinement**, ($N = 5$, $T = 1$ K)



Mean-field – Many-body

Mean-field, DFT

$$i\hbar d_t \rho(t) = [H[\rho(t)] + W(t), \rho(t)]$$

Hilbert space of single-electron states

Many-body

$$i\hbar d_t \rho(t) = [H + W(t), \rho(t)]$$

Fock-space of many-electron states constructed from the Hilbert space of single-electron states

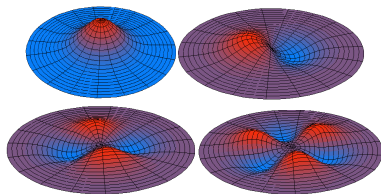
Operators in infinite spaces $\rightarrow$ infinite matrices $\rightarrow$ truncation

Mean-field: iterations...

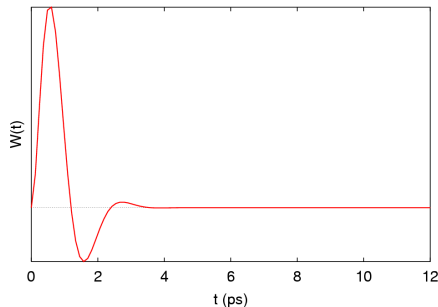
Time evolution

At $t = t_0$: $H(t) \rightarrow H + W(t)$

$$W(t) = V_t r^{|N_p|} \cos(N_p \phi) \exp(-sr^2 - \Gamma t) \sin(\omega_1 t) \sin(\omega t) \theta(\pi - \omega_1 t)$$



- $N_p = 0, \pm 1, \pm 2, \pm 3$
- $sa_w^2 = 1.00$, $\Gamma = 2$ THz
- $\hbar\omega = 2.63$ meV, $\hbar\omega_1 = 0.658$ meV



Nonequilibrium evolution

$$i\hbar d_t \rho(t) = [H + W(t), \rho(t)].$$

$$\begin{aligned} i\hbar \dot{T}(t) &= H(t) T(t) \\ -i\hbar \dot{T}^+(t) &= T^+(t) H(t) \end{aligned}$$

$$\rho(t + \Delta t) = T(\Delta t) \rho(t) T^+(\Delta t)$$

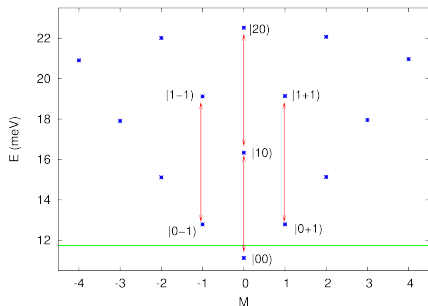
Crank-Nicholson + iteration

$$\left\{ 1 + \frac{i\Delta t}{2\hbar} H[\rho; t + \Delta t] \right\} T(\Delta t) \approx \left\{ 1 - \frac{i\Delta t}{2\hbar} H[\rho; t] \right\}$$

No assumption about Fermi-distribution, except at $t = 0$

Monopole excitation - breathing mode

LDA Kohn-Sham energies



Quantum dot, two electrons

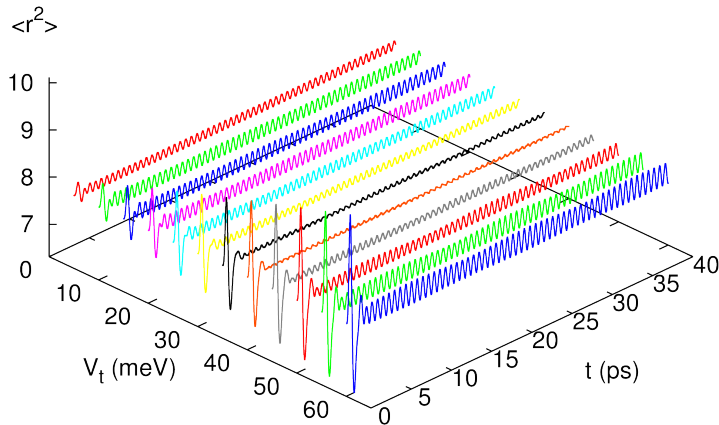
Confinement

$$V_{\text{par}}(r) = \frac{1}{2} m^* \omega_0^2 r^2$$

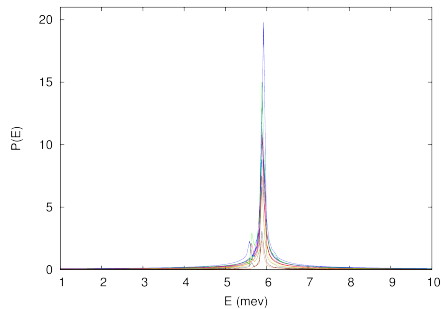
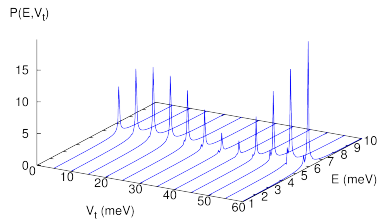
Central hill

$$V_c(r) = V_0 \exp(-\gamma r^2)$$

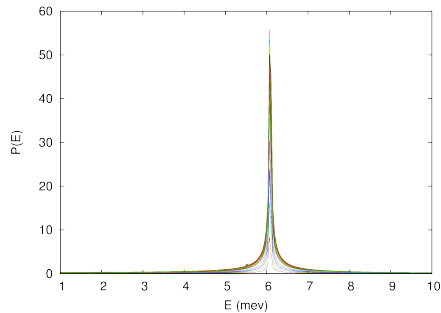
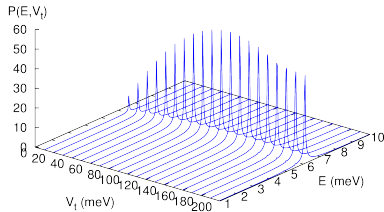
DFT, central hill



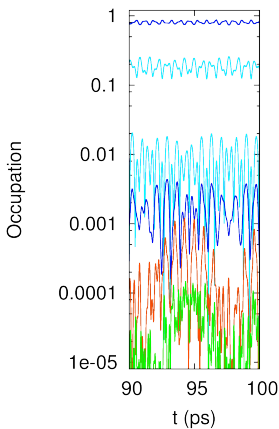
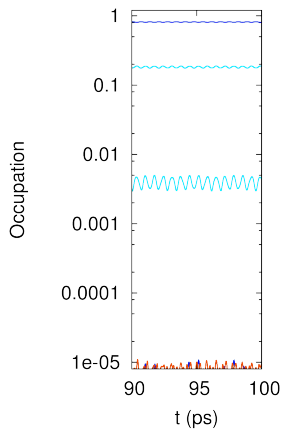
DFT, central hill, Fourier spectra



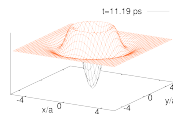
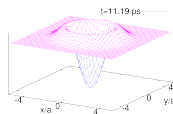
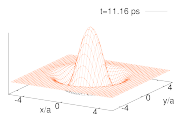
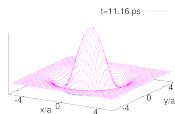
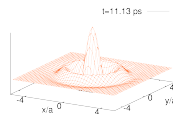
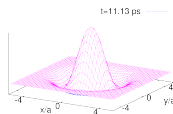
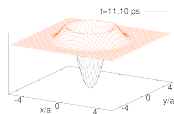
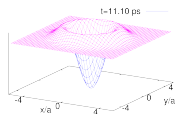
Hartree, central Hill, Fourier spectra



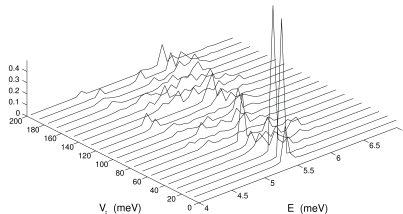
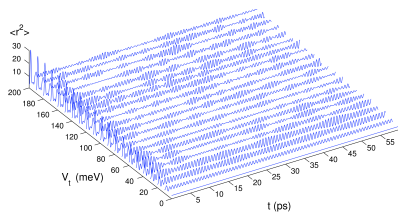
Hartree, occupation, $V_t = 10, \quad 200 \text{ meV}$



DFT, induced density, central hill, $V_t = 35$ meV

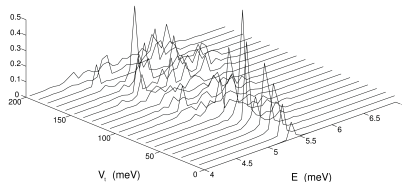
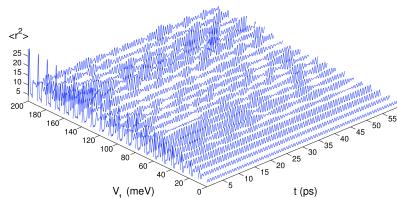


Nonlinear Schrödinger-Poisson, no central hill



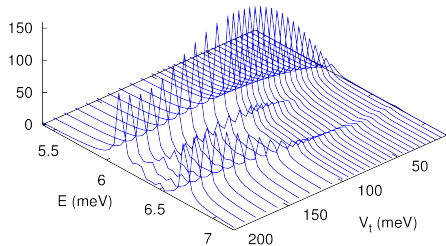
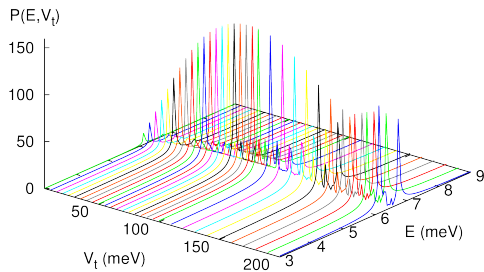
Direct solution, no iteration

Nonlinear Schrödinger-Poisson, central hill

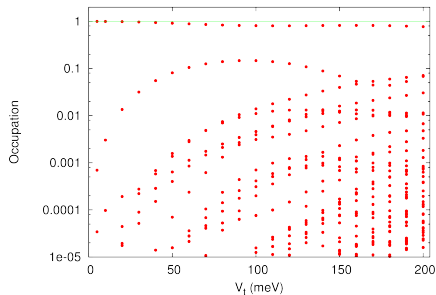
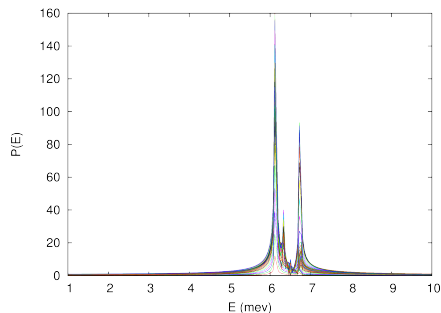


Direct solution, no iteration

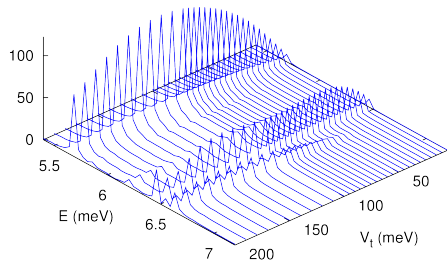
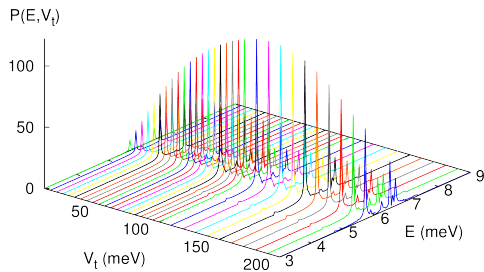
Exact, no central hill, Fourier spectra



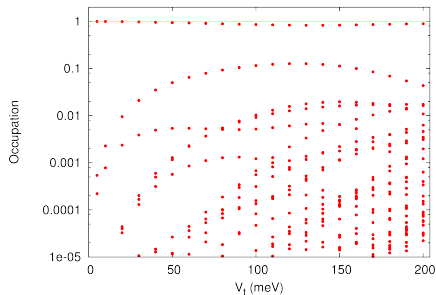
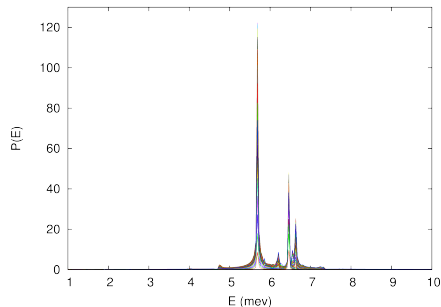
Exact, no central hill, Fourier spectrum, occupation



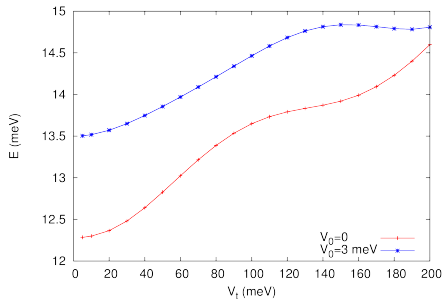
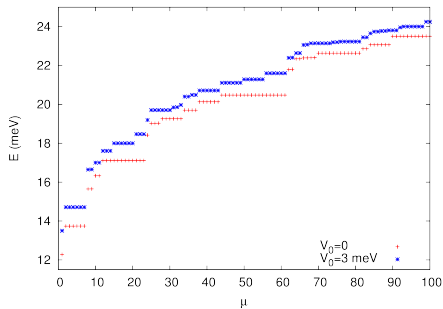
Exact, central hill, Fourier spectra



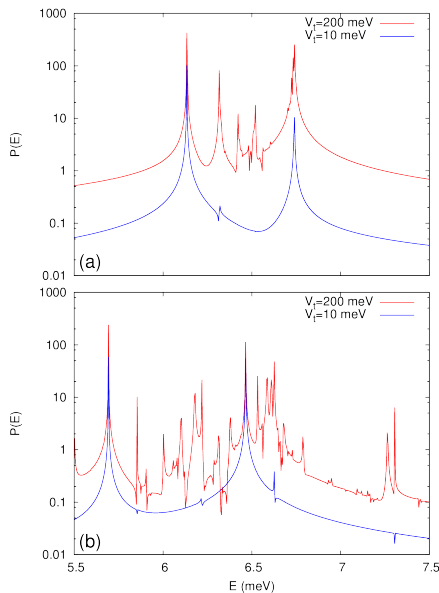
Exact, central hill, Fourier spectrum, occupation



Exact, two-electron spectra, total energy



Exact, Fourier spectra, no hill, hill



- Exact: GPU-CUDA
- Exact: Static: 16836 2e states, Dynamic: 2415 2e states
- Exact: Time-evolution totally on the GPU Nvidia M2090
- DFT: Difficult to stabilize...
- Nonlinear behavior
 - Exact + Hartree + DFT: Peak height, in-energy
 - Nonlinear + iteration: Connection to higher order methods, orthogonal states
 - Nonlinear + direct sol: Nonlinear, not found in exact, nonorthogonal states
 - Different communities...