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

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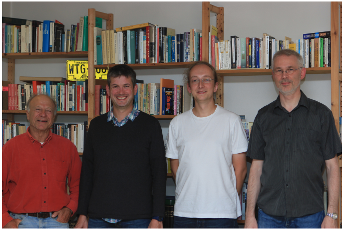

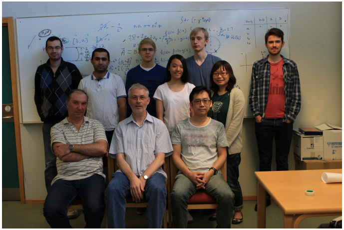

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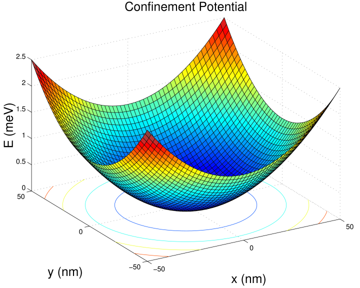
`http://arxiv.org/abs/1311.3252`

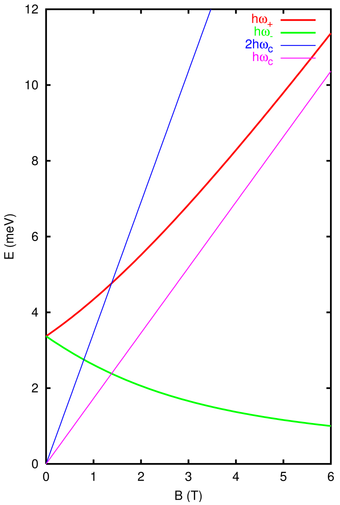
Background, (P.A. Maksym and T. Chakraborty, Phys. Rev. Lett. 65, 108 (1990))

Kohn's theorem

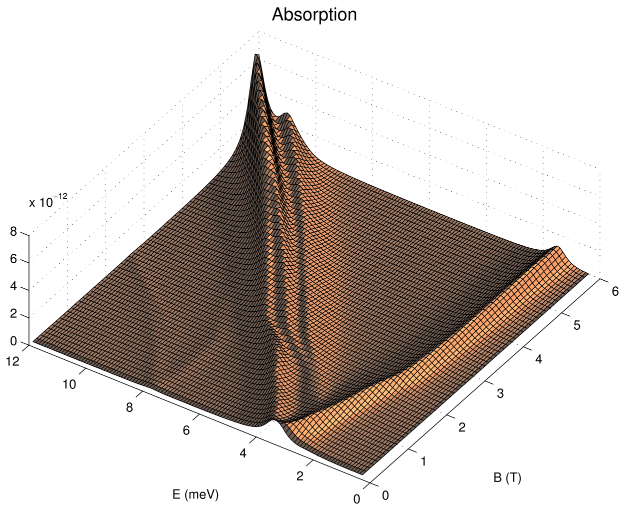
- Exact
- FIR-radiation, dipole
- Parabolic confinement

→ Only stiff CM-motion





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

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

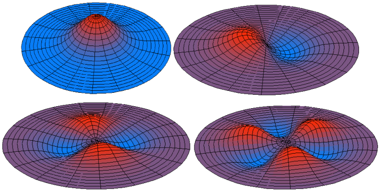
Fock-space of many-electron states constructed from the Hilbert space of single-electron states

Operators in infinite spaces → infinite matrices → truncation
Linear algebra

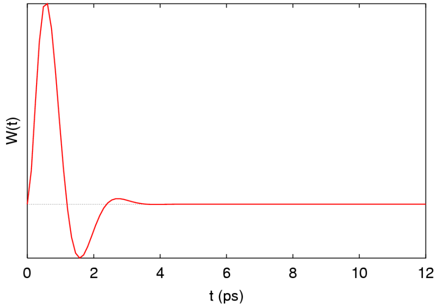
Time evolution

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

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



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



Nonequilibrium evolution

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

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

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

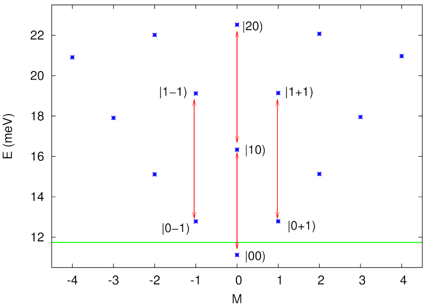
Crank-Nicholson + iteration

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

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

Monopole excitation - breathing mode

LDA Kohn-Sham energies



Quantum dot, two electrons

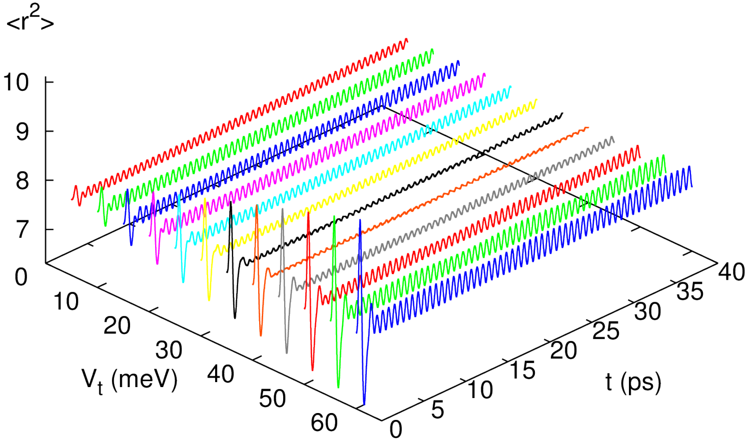
Confinement

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

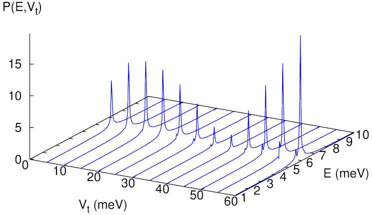
Central hill

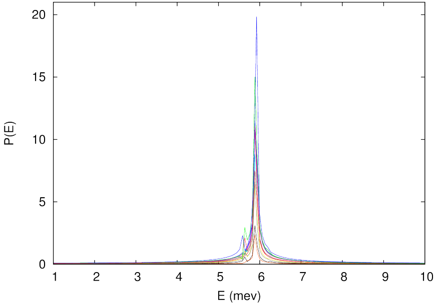
$$V_{\rm c}(r) = V_0 \exp\left(-\gamma r^2\right)$$

DFT, central hill

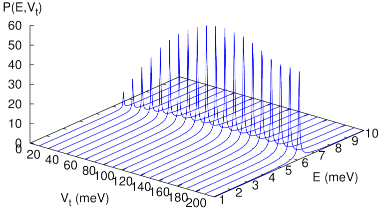


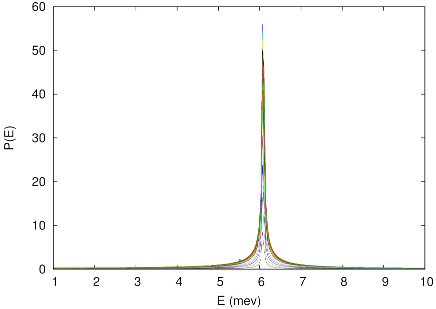
DFT, central hill, Fourier spectra



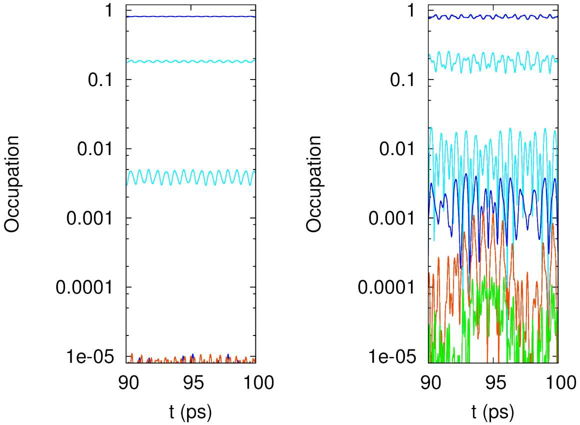


Hartree, central Hill, Fourier spectra

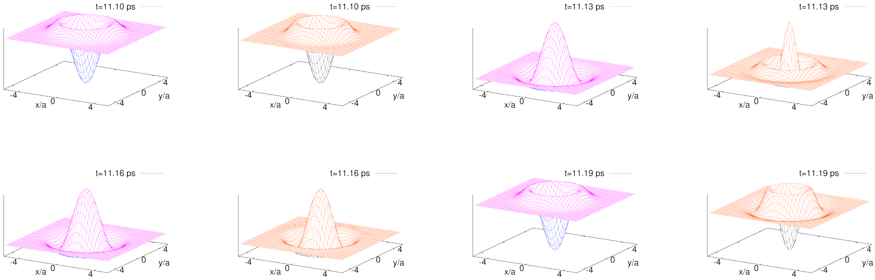




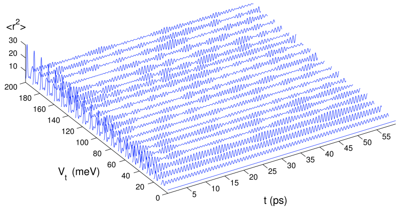
Hartree, occupation, $V_t = 10$, 200 meV

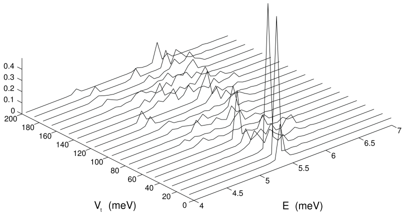


DFT, induced density, central hill, $V_t = 35$ meV



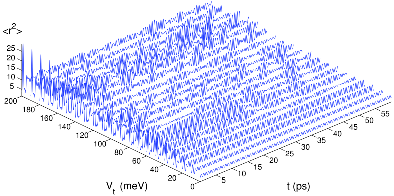
Nonlinear Schrödinger-Poisson, no central hill

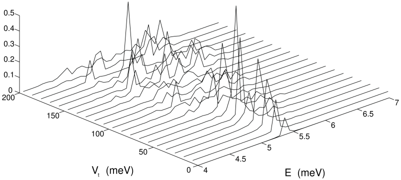




Direct solution, no iteration

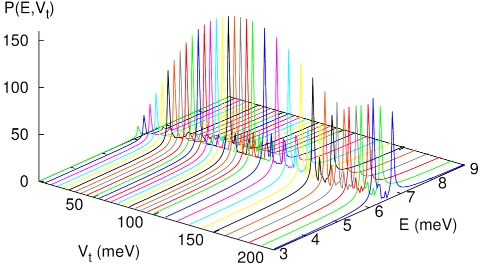
Nonlinear Schrödinger-Poisson, central hill

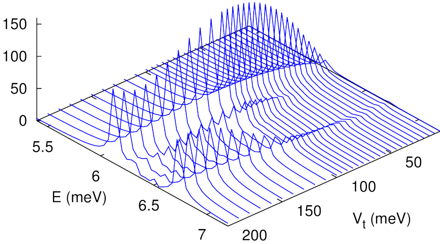




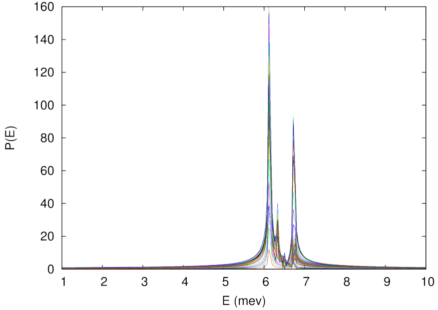
Direct solution, no iteration

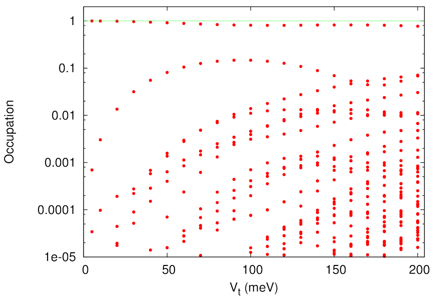
Exact, no central hill, Fourier spectra



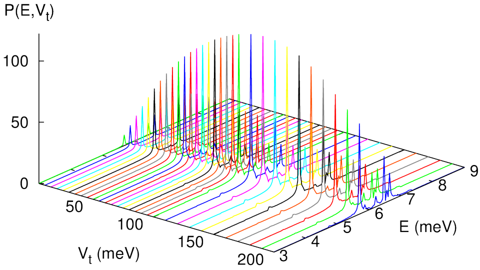


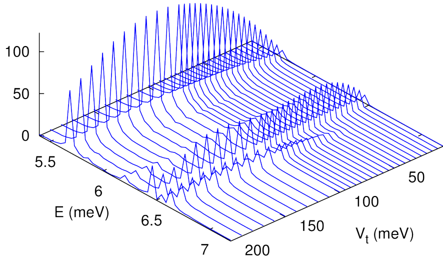
Exact, no central hill, Fourier spectrum, occupation



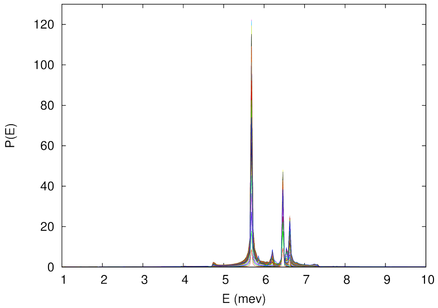


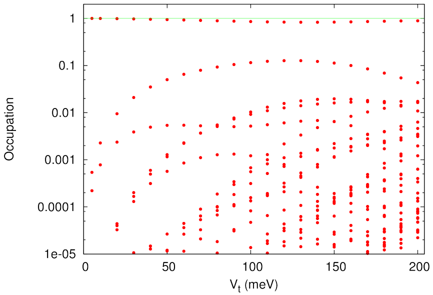
Exact, central hill, Fourier spectra



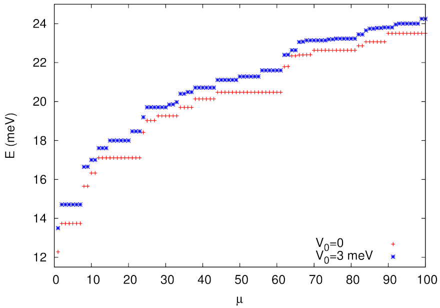


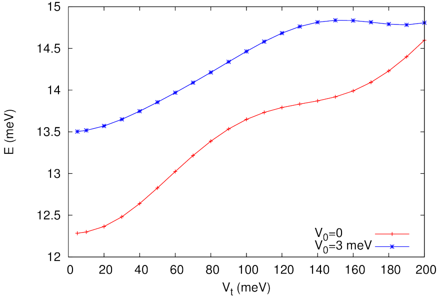
Exact, central hill, Fourier spectrum, occupation



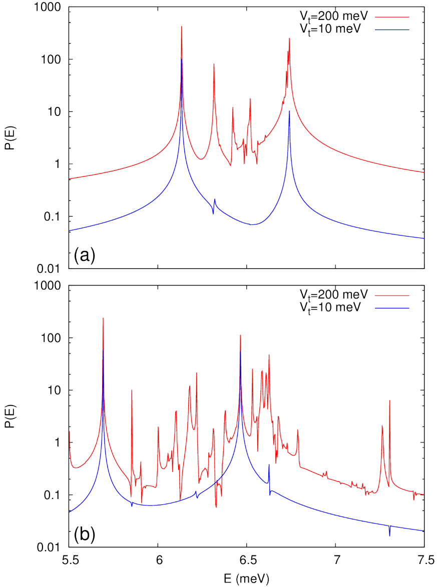


Exact, two-electron spectra, total energy





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...