Time-dependent phenomena in a quantum dot

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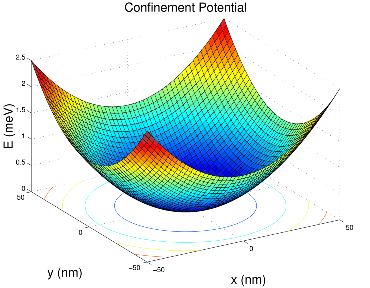
http://hartree.raunvis.hi.is/∼vidar/Rann/Fyrirlestrar/t-QD-UH.pdf

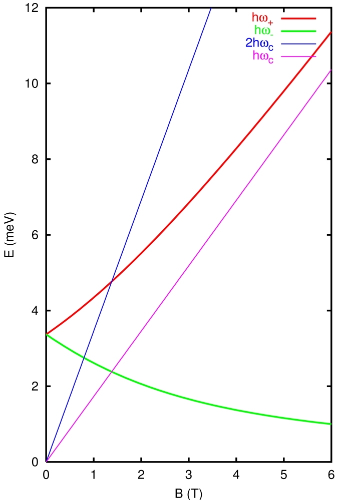
Background, (P.A. Maksym and T. Chakraborty, Phys. Rev. Lett. 65, 108 (1990))

Kohn's theorem

- Exact
- FIR-radiation
- Parabolic confinement

$\longrightarrow$ Only stiff CM-motion

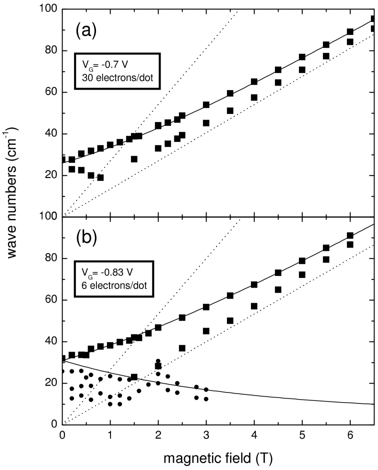




Experiments, (R. Krahne et al., Phys. Rev. B63, 195303 (2001))

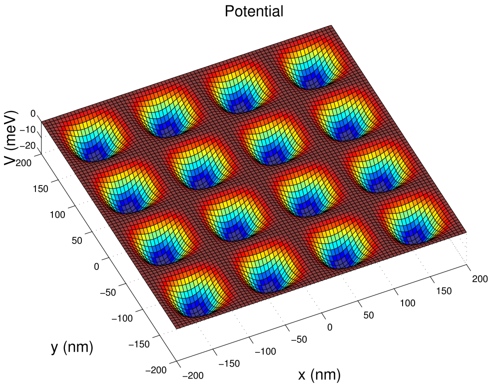
R. Krahne, D. Heitmann

- 6 or 30 electrons
- Mode below the upper Kohn mode



How is the confining potential in field induced dots?

- Must soften for large radii
- Periodic potential + $\mathbf{B}$ $\rightarrow$ trouble



Try some potentials for single dots

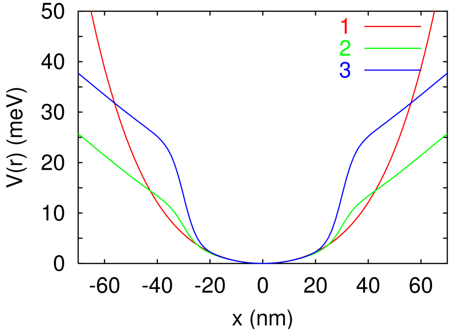
Parabolic + higher terms...

↓

excitations above the upper Kohn mode

+

Bernstein modes



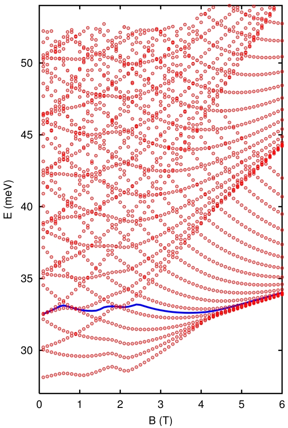
Self-consistent approach for interacting system

- Ground state:
  - Each electron interacts with the total electron density
- Excited state, (linear response):
  - The total electric field (in the FIR):
    $\mathbf{E}_{\rm tot} = \mathbf{E}_{\rm ext} + \mathbf{E}_{\rm ind}(\mathbf{E}_{\rm tot})$
- Consistency + self-consistency

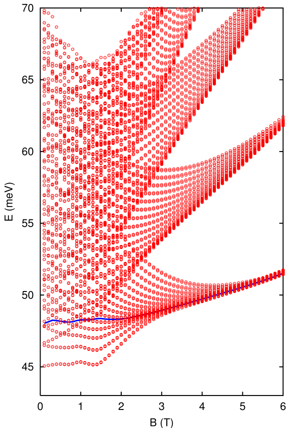
(Hartree-approximation, no spin)

V.G. and R.R.G., Phys. Rev. B43, 12098 (1991)

Darwin-Fock diagrams with interaction, $T = 1$ K

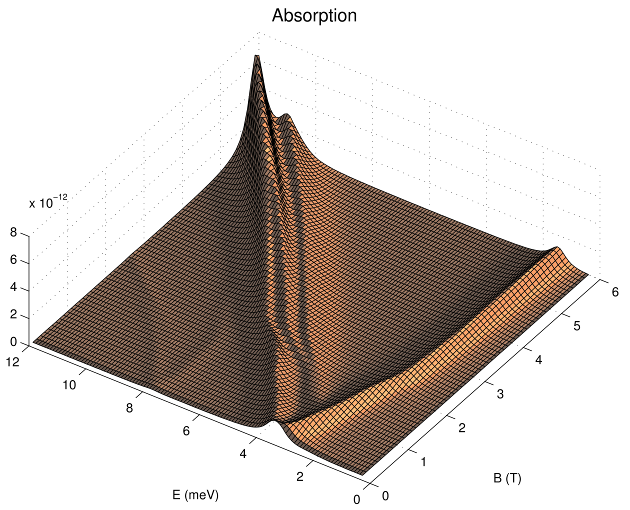


$N = 5$, no spin, $\alpha r^2 + \beta r^4$



$N = 10$, spin, αr^2 + softening

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



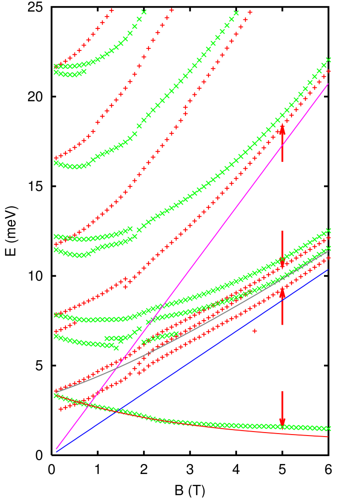
Calculated dispersion

Collective oscillations

$N = 5, \ T = 1$ K

- Left, right circular polarization
- Onset of Bernstein modes (class.)

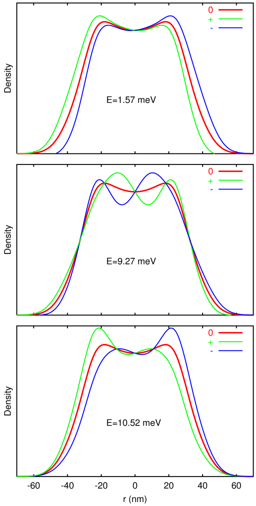
Phys. Rev. B51, 17744 (1995)



Induced density

Collective modes

- Mode recognition
- CM $\leftrightarrow$ relative motion



Open physics questions

- How does shape influence absorption?
- What happens beyond linear response?
- Time-dependent phenomena, transients?

Ground state

- Confined closed system of several 2D electrons
- General shape, ring, circular, elliptic, square, triangular dot …
- External constant perpendicular magnetic field

Time evolution

- Weak $\longrightarrow$ strong perturbation, general shape in time and space
- Nonequilibrium evolution
- Non-adiabatic
- Transients
- No dissipation

Ground state

$$H|\alpha) = (H_0 + H_\sigma + V_\phi + H_{\rm int})\,|\alpha) = \varepsilon_\alpha|\alpha),$$

$$V_\phi(\mathbf{r}) = \frac{1}{2}m^*\omega_0 r^2\sum_{p=1}^{p_{\rm max}}\alpha_p\cos(p\varphi) + V_0\exp(-\gamma r^2),$$

H_0 includes $\mathbf{B} = B\hat{\mathbf{z}}$ and $V_{\rm conf}(r) = m^*\omega_0^2 r^2/2$

Zeeman energy: $H_\sigma = \pm(1/2)g^*\mu_B B$

Length scale: $l = \sqrt{\hbar c/(eB)} \longrightarrow a = l\sqrt{\omega_c/\Omega}$

Energy scale: $\hbar\omega_c = \hbar eB/(m^*c) \longrightarrow \hbar\Omega = \hbar\sqrt{\omega_c^2 + 4\omega_0^2}$

DFT - ground state

Grid-free LSDA

- $\{n_\downarrow(\mathbf{r}),\ n_\uparrow(\mathbf{r})\} \to \{\tilde{\nu}(\mathbf{r}),\ \zeta(\mathbf{r})\}$
- Fock-Darwin basis $\{\phi_{nM}\}$ + statistical operator $\hat{\rho}$
  $\to$ matrix elements of ν and ζ
- All functionals are functionals of the matrices $\tilde{\nu}$ and ζ

- Y.C. Zheng and J. Almlöf, Chem. Phys. Lett. 214, 397 (1993)
- G. Berghold, J. Hutter, and M. Parrinello, Theor. Chem. Acc. 99, 344 (1998)
- K.R. Glaesemann and M.S. Gordon, J. Chem. Phys. 110, 6580 (1999)

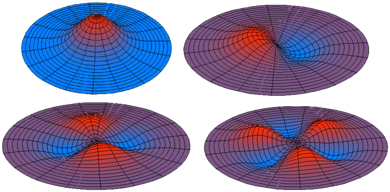
Functionals and parametrization

- M. Koskinen, et al., Phys. Rev. Lett. 79, 1389 (1997)
- U. von Barth and B. Holm, Phys. Rev. B 54, 8411 (1996)
- B. Tanatar and D.M. Ceperley, Phys. Rev. B 39, 5005 (1989)

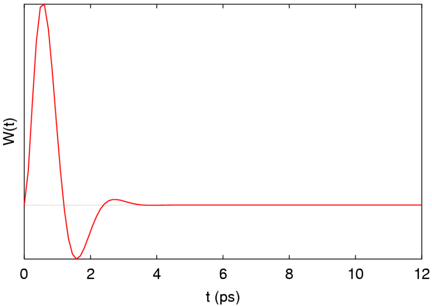
Time evolution

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

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



- $N_p = 0, \pm1, \pm2, \pm3$
- $s = 0$, $\Gamma = 2$ THz
- $\omega = 4$ THz, $\omega_1 = 1$ THz



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 $t = 0$

Magnetization

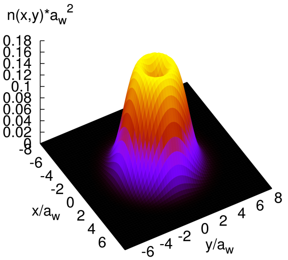
$$\mathcal{M}_o(t) = -\frac{e}{2c}\mathrm{tr}\{(\mathbf{r}\times\dot{\mathbf{r}})\cdot\hat{\mathbf{z}}\,\rho(t)\}$$

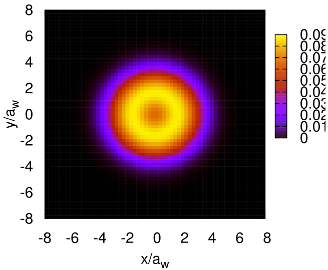
Technical implementation

- Fock-Darwin basis $\{\phi_{nM}\} \longrightarrow$
- Analytical matrix elements
- Grid-free LSDA, compact "small" matrices
- Complicated LSDA potentials $\longrightarrow$ complicated functions of $\tilde{\nu}$ $\longrightarrow$ heavy matrix multiplication
- F95 $\longrightarrow$ easy parallelization on multicore machines
- Phys. Rev. B67, 161301(R) (2003), Phys. Rev. B68, 165343 (2003)

Circular quantum dot

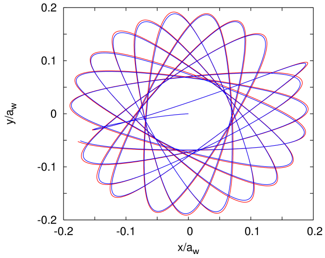
- Circular dot
- $N = 6$
- $B = 0.6$ T
- $T = 4$ K



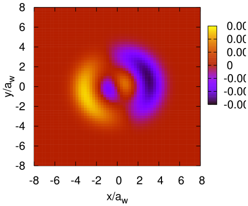


Dipole excitation

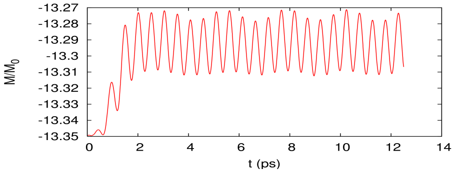
Center of mass



Induced density, ($t = 12.5$ ps, 5000 steps)



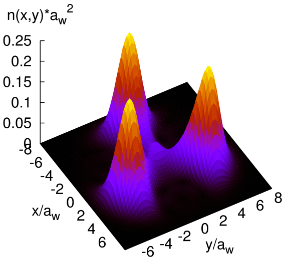
Magnetization

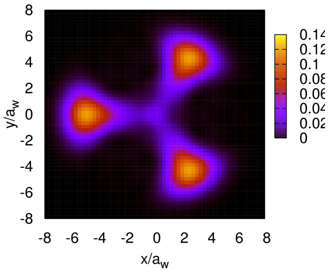


- No energy flows into internal modes
- Kohn's theorem

Triangular quantum dot

- Triangular dot, $\alpha_3 = 0.7$
- $N = 6$
- $B = 0.6$ T
- $T = 1$ K

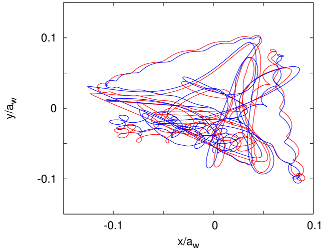




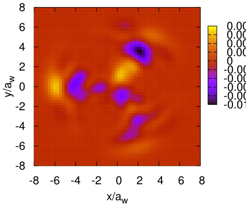
- Kohn's theorem does not hold
- Energy will flow into internal modes, transient time?

Dipole excitation

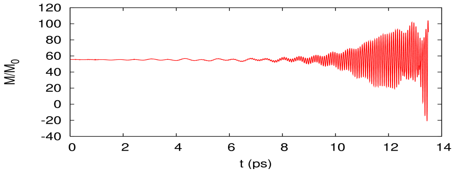
Center of mass



Induced density, $(t = 13.5$ ps, 9000 steps)

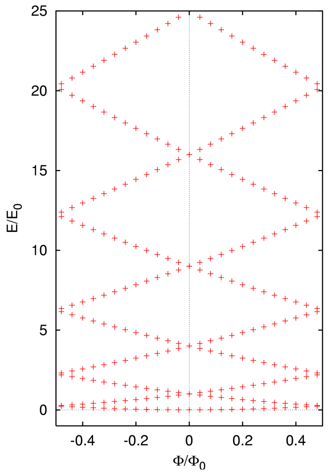


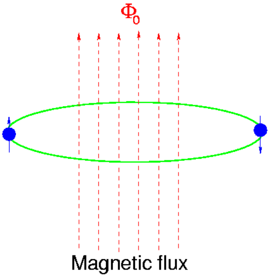
Magnetization



- Energy pumped into relative modes
- long transient time
- Spin modes

1D quantum ring



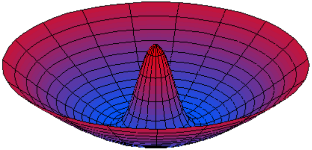


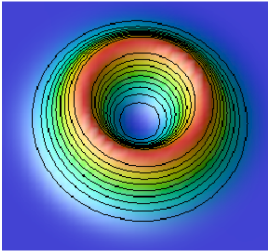
The magnetic flux can be gauge transformed away resulting in a "twisted boundary condition" $\psi(\phi + 2\pi) = \psi(\phi)\exp(i2\pi\Phi/\Phi_0)$.

$$\mathcal{E}_M = \frac{\hbar^2}{2m^* R^2}\left(M - \frac{\Phi}{\Phi_0}\right)^2$$

Quantum ring

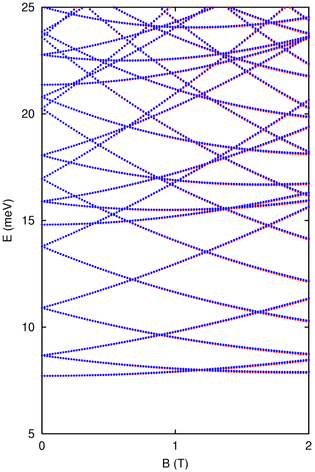
Confinement, density





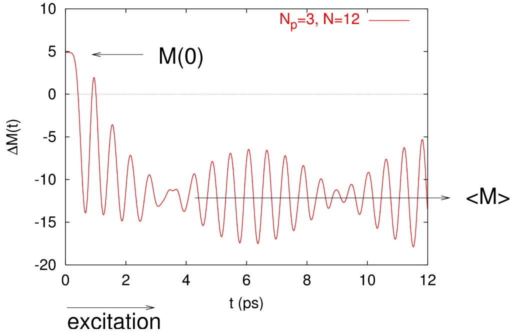
$N = 12$

Noninteracting single-electron spectrum



Quantum ring

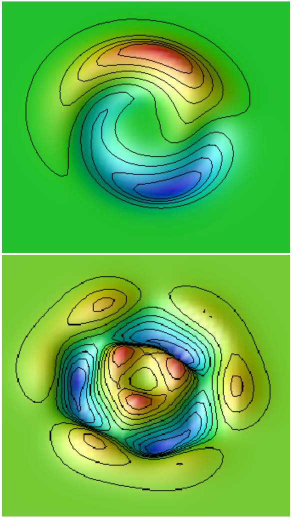
Dynamic orbital magnetization



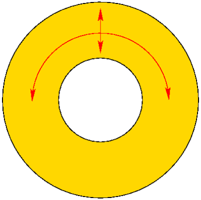
- $B = 0.6$ T
- $T = 1.0$ K
- $V_t a^3 = 1.0$ meV
- In units of $M_0 = \mu_B$
- ΔM: dynamic

Strong excitation reverses the persistent current

Induced density, $N_p = 1$, $N_p = 3$, $B = 0.6$ T



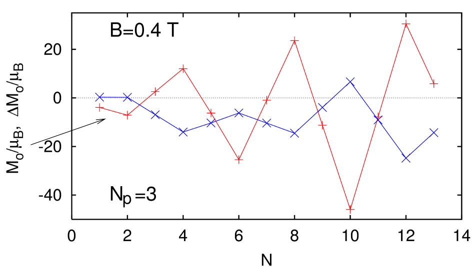
Lorentz-force



- No current excited at $B = 0$ T
- No current for $N_p = 0$
- Collective radial mode + symmetry breaking of pulse → nonequilibrium state with different persistent current
- Happens only in ring of finite width

Variation with N

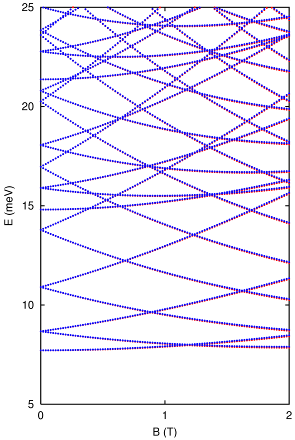
Dynamic and static magnetization



Thermodynamically in equilibrium

$$\mathcal{M} = -\frac{\partial F}{\partial B}$$

Single-electron spectrum



Conclusions

- Flexible model
- Model of strong excitation → time evolution into nonequilibrium states
- Transient effects
- Manipulation of currents in a ring, (see E. Räsänen et al. PRL 98 157404 (2007))
- Dissipation, (G. Piacente and G. Q. Hai, PRB 75, 125324 (2007))
- Comparison to present work on time-dependent transport, (cond-mat/0703179)

Cooworkers

- Chi-Shung Tang, Andrei Manolescu, Llorenç Serra, Marian Nita
- Roman Krahne, Detlef Heitmann
- Ingibjörg Magnúsdóttir, Sigríður Sif Gylfadóttir, Sigurður I. Erlingsson