Time-dependent phenomena in a quantum dot

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Criteria

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 → strong perturbation, general shape in time and space
- Nonequilibrium evolution
- Adiabatic
- No dissipation

Grid-free LSDA

- 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)

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

Density: $n = n_\uparrow + n_\downarrow \longrightarrow \tilde{\nu}(\mathbf{r}) = 2\pi a^2 n(\mathbf{r})$ effective filling factor

Polarization: $\zeta(\mathbf{r}) = [n_\uparrow(\mathbf{r}) - n_\downarrow(\mathbf{r})]/n(\mathbf{r})$

DFT - ground state

Change of variables

$$V_{xc,\sigma}(\mathbf{r},B) = \frac{\partial}{\partial n_\sigma}\left(n\epsilon_{xc}[n_\uparrow, n_\downarrow, B]\right)\Big|_{n_\sigma = n_\sigma(\mathbf{r})},$$

$$\Downarrow$$

$$V_{xc,\uparrow} = \frac{\partial}{\partial\tilde{\nu}}(\tilde{\nu}\epsilon_{xc}) + (1-\zeta)\frac{\partial}{\partial\zeta}\epsilon_{xc}$$

$$V_{xc,\downarrow} = \frac{\partial}{\partial\tilde{\nu}}(\tilde{\nu}\epsilon_{xc}) - (1+\zeta)\frac{\partial}{\partial\zeta}\epsilon_{xc}$$

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)

Grid-free LSDA

Use a basis

$$|\alpha) = \sum_{\beta} c_{\alpha\beta}|\beta\rangle, \quad \psi_\alpha(\mathbf{r}) = \sum_{\beta} c_{\alpha\beta}\phi_\beta(\mathbf{r})$$

$$\langle\alpha|\tilde{\nu}|\beta\rangle = \sum_{p,q} \rho_{qp} \int d\mathbf{r}\; \phi_\alpha^*(\mathbf{r})\phi_p^*(\mathbf{r})\phi_q(\mathbf{r})\phi_\beta(\mathbf{r})$$

$$\rho_{qp} = \sum_{\gamma} f(\varepsilon_\gamma - \mu) c_{\gamma p}^* c_{\gamma q}$$

$$\langle\alpha|\zeta|\beta\rangle = \sum_{\gamma} \langle\alpha|(\tilde{\nu}_\uparrow - \tilde{\nu}_\downarrow)|\gamma\rangle\langle\gamma|\tilde{\nu}^{-1}|\beta\rangle$$

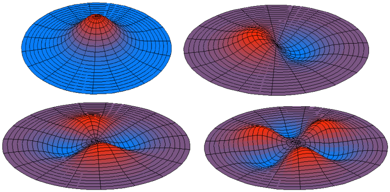
$$\tilde{\nu} = \mathbf{U}\;\mathbf{diag}(\lambda_1, \cdots, \lambda_n)\mathbf{U}^+$$

$$\mathbf{f}[\tilde{\nu}] = \mathbf{U}\;\mathbf{diag}\left(f(\lambda_1), \cdots, f(\lambda_n)\right)\mathbf{U}^+.$$

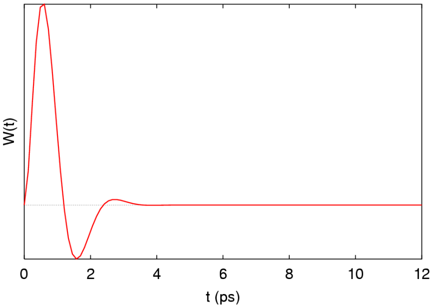
Time evolution

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

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



- $N_p = 0, \pm 1, \pm 2, \pm 3$
- $s = 0$, $\Gamma = 2$ 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

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

Magnetization

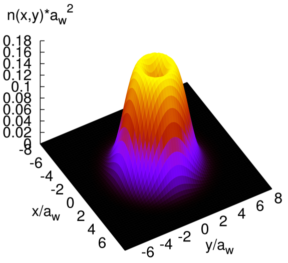
$$\mathcal{M}_o(t) = -\frac{e}{2c} \mathrm{tr}\{(\mathbf{r} \times \dot{\mathbf{r}}) \cdot \hat{\mathbf{z}}\ \rho(t)\}$$

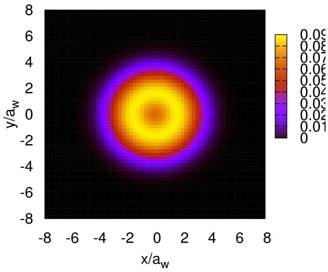
Technical implementation

- Fock-Darwin basis $\{\phi_\alpha\} \rightarrow$
- Analytical matrix elements
- Grid-free LSDA, compact "small" matrices
- Complicated LSDA potentials $\rightarrow$ complicated functions of $\tilde{\nu}$ $\rightarrow$ heavy matrix multiplication
- F95 $\rightarrow$ easy parallelization on multicore machines

Circular quantum dot

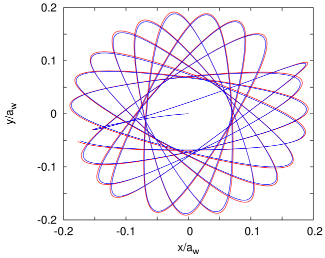
- Circular dot
- $N = 6$
- $B = 0.6$ T
- $T = 4$ K



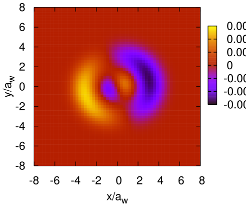


Dipole excitation

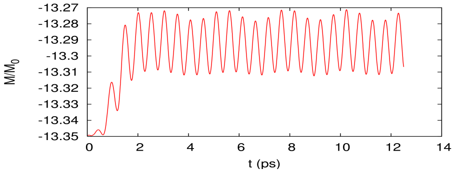
Center of mass



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



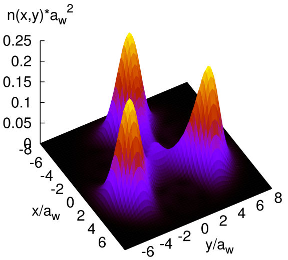
Magnetization

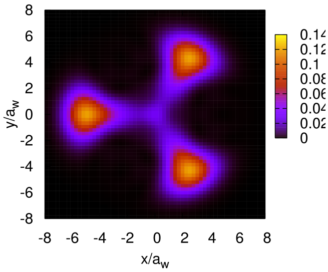


- No energy flows into internal modes
- Kohn's theorem

Triangular quantum dot

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

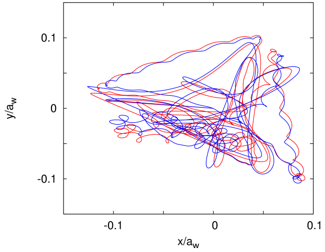




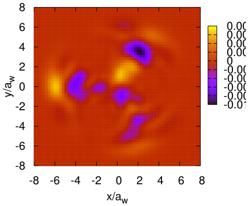
- Kohn's theorem does not hold
- Energy will flow into internal modes, transient time?

Dipole excitation

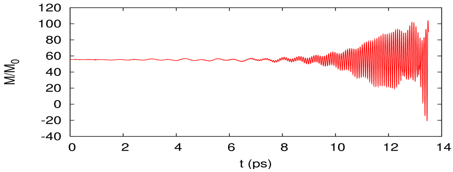
Center of mass



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

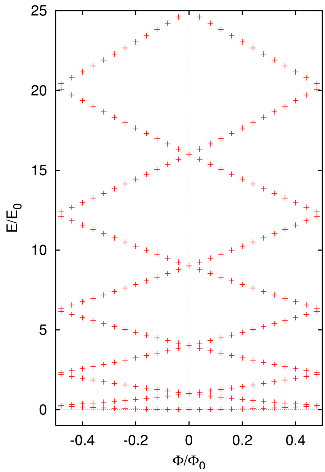


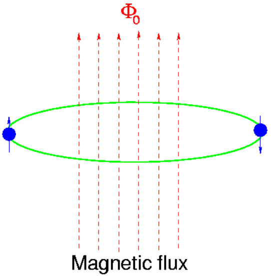
Magnetization



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

1D quantum ring



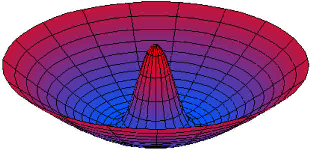


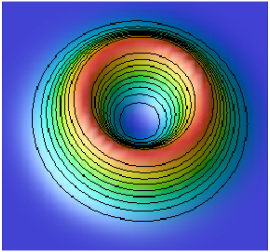
The magnetic flux can be gauge transformed away resulting in a "twisted boundary condition" $\psi(\phi + 2\pi) = \psi(\phi)\exp(i2\pi\Phi/\Phi_0)$.

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

Quantum ring

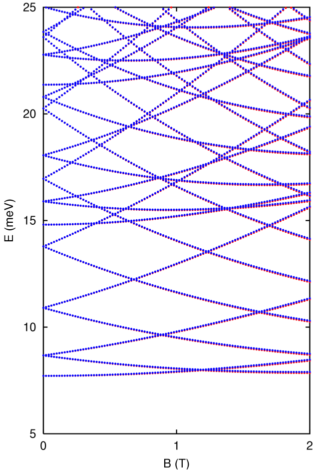
Confinement, density





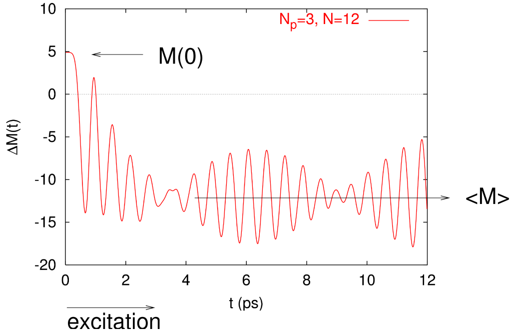
$N = 12$

Noninteracting single-electron spectrum



Quantum ring

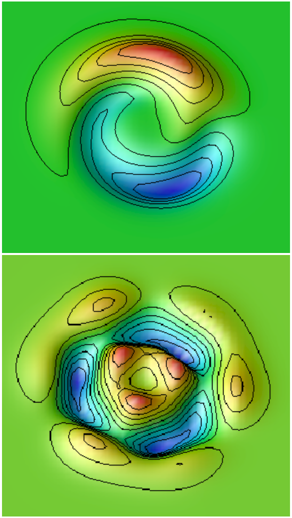
Dynamic orbital magnetization



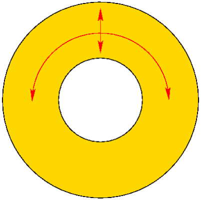
- $B = 0.6$ T
- $T = 1.0$ K
- $V_t a^3 = 1.0$ meV
- In units of $M_0 = \mu_B$
- ΔM: dynamic

Strong excitation reverses the persistent current

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



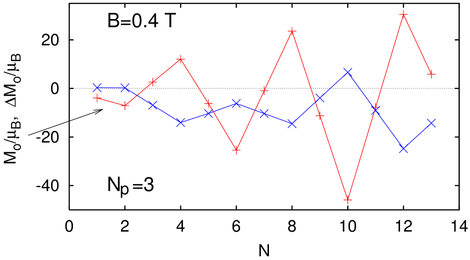
Lorentz-force



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

Variation with N

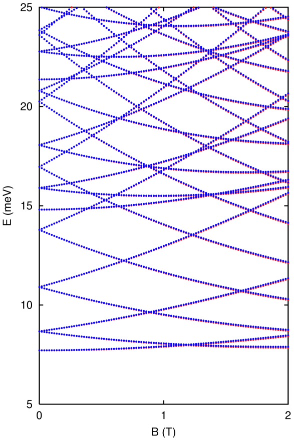
Dynamic and static magnetization



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)

Publications

- Phys. Rev. B67, 161301(R) (2003)
- Phys. Rev. B68, 165343 (2003)
- Physica E 27, 278 (2005)