Numerically exact diagonalization applied to time-evolution of small closed or open many-body systems

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NORDITA, September, 2014

Cooperation

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- *New Journal of Physics* **11**, 073019 (2009)
- *New Journal of Physics* **11**, 113007 (2009)
- *Phys. Rev. B* **81**, 155442 (2010)
- *Phys. Rev. B* **81**, 205319 (2010)
- *New Journal of Physics,* **14**, 013036 (2012)
- *Phys. Rev. B* **85**, 075306 (2012)
- *Fortschritte der Physik* **61**, no 2-3, 305 (2013)
- *Annalen der Physik* **526**, 235 (2014)

. . . and more, see:

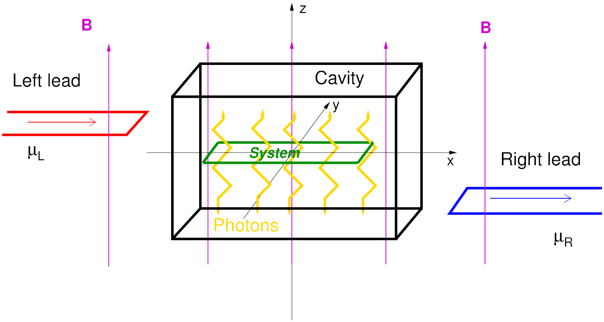
`http://hartree.raunvis.hi.is/~vidar/Rann/rit/node1.html`

Open system

- Central system
  - Non trivial geometry $\rightarrow$ complicated spectrum
  - Coulomb interaction, exact
  - Photon cavity - para- and diamagnetic interaction, exact...
- External leads, electron reservoirs
  - Geometric coupling
- External magnetic field
- Non-Markovian, memory effects, time-evolution

Approach

$$H(t) = \underbrace{\underbrace{\underbrace{H_{\mathrm{e}} + H_{\mathrm{Coul}}}_{\text{diagonalize+cut}} + H_{\mathrm{EM}} + H_{\mathrm{e-EM}}}_{\text{diagonalize+cut}\rightarrow H_{\mathrm{S}}} + H_{\mathrm{LR}} + H_{\mathrm{T}}(t)}_{\text{project on system}(H_{\mathrm{S}})\rightarrow\text{GME}}$$



e-EM coupling

Full electron-photon coupling

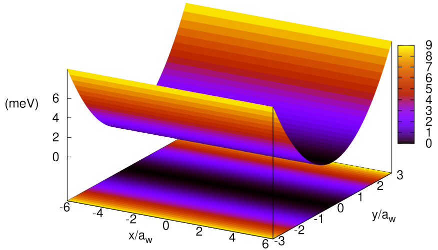
$$
\begin{aligned}
&\int d\mathbf{r}\ \psi^\dagger \left\{ \frac{1}{2m^*}\left(-i\hbar\nabla + \frac{e}{c}\left[\mathbf{A} + \mathbf{A}_{\rm ext}\right]\right)^2 \right\}\psi \\
&= \int d\mathbf{r}\ \psi^\dagger \left\{ \frac{1}{2m^*}\left(-i\hbar\nabla + \frac{e}{c}\mathbf{A}\right)^2 \right\}\psi \\
&- \frac{1}{c}\int d\mathbf{r}\ \mathbf{j}\cdot\mathbf{A} - \frac{e^2}{2m^* c}\int d\mathbf{r}\ \rho A^2 \\
&= H_{\rm e} + H_{\rm e-EM}
\end{aligned}
$$

$$
\mathbf{j} = -\frac{e}{2m^*}\left\{\psi^\dagger\left(\boldsymbol{\pi}\psi\right) + \left(\boldsymbol{\pi}^*\psi^\dagger\right)\psi\right\}
$$

$$
\rho = -e\psi^\dagger\psi, \qquad \boldsymbol{\pi} = \left(\mathbf{p} + \frac{e}{c}\mathbf{A}_{\rm ext}\right)
$$

Central system, generic type

- Finite parabolic quantum wire $L_x = 300$ nm
- GaAs parameters



- External perpendicular magnetic field, $\mathbf{B} = B\hat{\mathbf{z}}$
  Confinement energy in y-direction $\hbar\Omega_0 = 1.0$ meV
- Semi-infinite leads in magnetic field, parabolic y-confinement

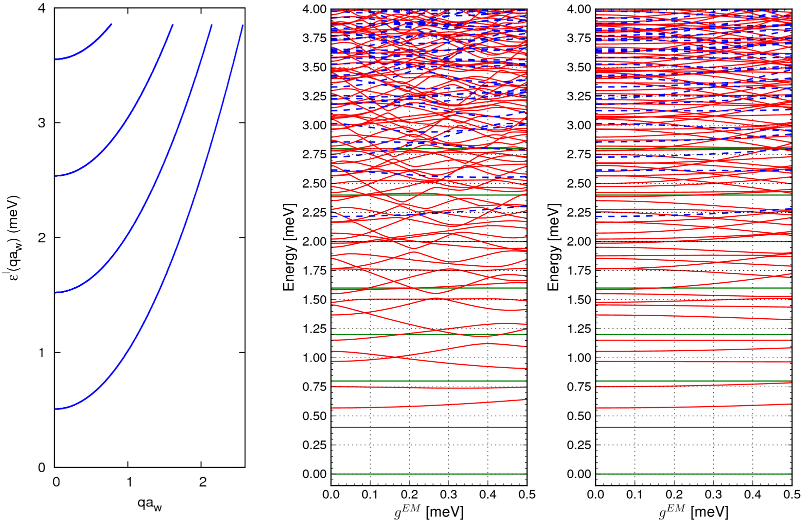
Single cavity mode

$$
\begin{aligned}
H_0 = &\sum_i E_i d_i^\dagger d_i + \hbar\omega a^\dagger a + \frac{1}{2}\sum_{ijrs}\langle ij|V_{\mathrm{Coul}}|rs\rangle d_i^\dagger d_j^\dagger d_s d_r \\
&+ \mathcal{E}_\mathrm{c}\sum_{ij} d_i^\dagger d_j\ g_{ij}\left\{a + a^\dagger\right\} \\
&+ \mathcal{E}_\mathrm{c}\left(\frac{\mathcal{E}_\mathrm{c}}{\hbar\Omega_w}\right)\sum_i d_i^\dagger d_i \left\{\left(a^\dagger a + \frac{1}{2}\right) + \frac{1}{2}\left(aa + a^\dagger a^\dagger\right)\right\}
\end{aligned}
\tag{1}
$$

$$
\begin{aligned}
H_0 = &\sum_\mu |\mu)\tilde{E}_\mu(\mu| + \hbar\omega a^\dagger a + g^{\mathrm{EM}}\sum_{\mu\nu ij}|\mu)\langle\mu|\mathcal{V}^+ d_i^\dagger d_j \mathcal{V}|\nu\rangle(\nu|\ g_{ij}\left\{a + a^\dagger\right\} \\
&+ g^{\mathrm{EM}}\left(\frac{g^{\mathrm{EM}}}{\hbar\Omega_w}\right)\sum_{\mu\nu i}|\mu)\langle\mu|\mathcal{V}^+ d_i^\dagger d_i \mathcal{V}|\nu\rangle(\nu|\left\{\left(a^\dagger a + \frac{1}{2}\right) + \frac{1}{2}\left(aa + a^\dagger a^\dagger\right)\right\}
\end{aligned}
$$

$$
\underbrace{|\mu) \otimes |N_{\mathrm{ph}}\rangle \longrightarrow |\mu)_{\mathrm{e-EM}}}_{\text{diagonalization}}
$$

Energy spectra, leads, e-EM central system x- and y-pol., $\hbar\nu = 0.4$ meV, $B = 0.1$ T



Opening the system to the leads → GME

- Weak coupling to leads
- Non-Markovian
- Memory effects
- $\mathcal{P} = \rho_L \rho_R \mathrm{Tr}_{LR}$
- $H_{\mathrm{T}}^l(t) = \chi^l(t) \sum_{q,a} \left\{ T_{qa}^l d_{ql}^\dagger c_a + (T_{qa}^l)^* c_a^\dagger d_{ql} \right\}$
- Reduced statistical operator $\rho_{\mathrm{S}}(t) = \mathcal{P}\{W(t)\}$

Liouville-von Neumann equation

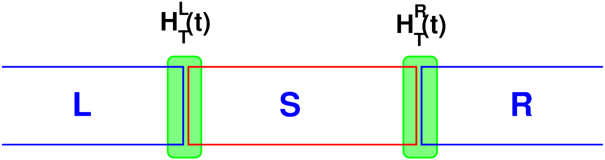
$$\dot{W}(t) = -\frac{i}{\hbar} [H(t), W(t)] = -i\mathcal{L} W(t)$$

$$\langle A(t) \rangle = \mathrm{Tr}\{W(t)A\} = \mathrm{Tr}_{\mathrm{S}}\{\rho_{\mathrm{S}}(t)A\}$$

$$i\hbar\dot{\rho}_{\mathrm{S}}(t) \approx \underbrace{\mathcal{L}_S \rho_{\mathrm{S}}(t)}_{\text{closed system}} + \underbrace{\frac{1}{i\hbar}\mathrm{Tr}_{LR}\left\{\mathcal{L}_T(t)\int_0^t ds\, e^{-i(t-s)\mathcal{L}_0}\mathcal{L}_T(s)\rho_L\rho_R\rho_{\mathrm{S}}(s)\right\}}_{\text{dissipation, memory}}$$

Coupling Hamiltonian

Contact area



Coupling tensor with sensitivity to geometry

$$T_{aq}^{l} = \int_{\Omega_S^l \times \Omega_l} d\mathbf{r}\, d\mathbf{r}' \left(\psi_q^l(\mathbf{r}')\right)^* \psi_a^S(\mathbf{r}) g_{aq}^l(\mathbf{r}, \mathbf{r}')$$

Nonlocal overlap

$$g_{aq}^l(\mathbf{r}, \mathbf{r}') = g_0^l \exp\left[-\delta_1^l (x - x')^2 - \delta_2^l (y - y')^2\right] \exp\left(\frac{-|E_a - \epsilon^l(q)|}{\Delta_E^l}\right)$$

Basis transformations

Transform the coupling tensor into the Coulomb interacting many-electron basis $\{|\mu)\}$ and the electron-photon basis $\{|\breve{\mu})\}$

$$\tilde{\mathcal{T}}^l(q) = \mathcal{W}^+\mathcal{V}^+\mathcal{T}^l(q)\mathcal{V}\mathcal{W}, \quad \left(\tilde{\mathcal{T}}^l(q)\right)^* = \mathcal{W}^+\mathcal{V}^+\left(\mathcal{T}^l(q)\right)^*\mathcal{V}\mathcal{W}$$

and the rest of the Hamiltonian after each diagonalization

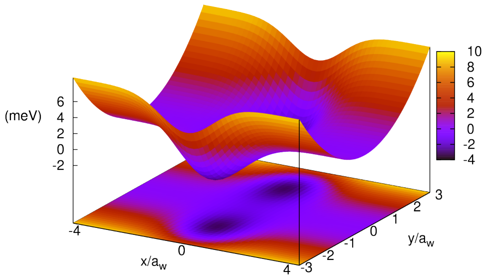
- Fock space construction and truncation schemes

Step by step guide

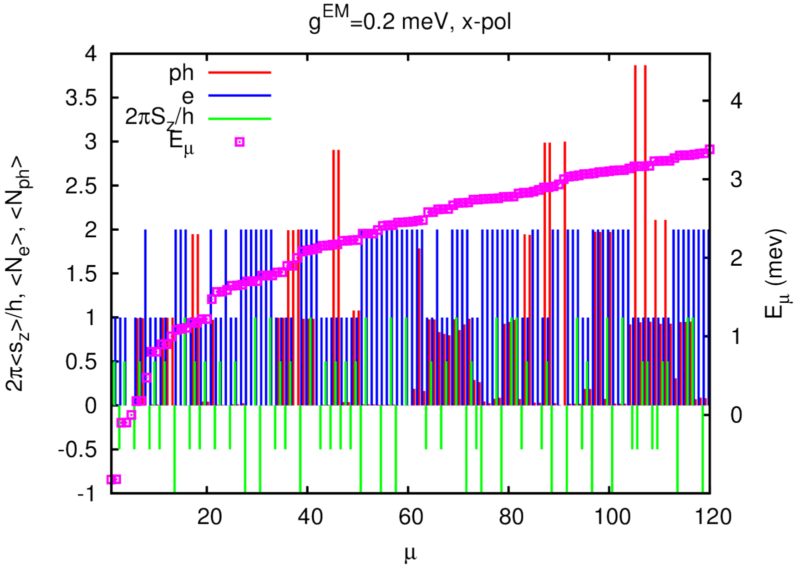
- http://hartree.raunvis.hi.is/~vidar/Nam/TE/GME-1.pdf
- http://hartree.raunvis.hi.is/~vidar/Nam/TE/GME-2.pdf
- http://hartree.raunvis.hi.is/~vidar/Nam/TE/GME-3.pdf
- http://hartree.raunvis.hi.is/~vidar/Nam/TE/GME-4.pdf

Specific central system, embedded parallel dots

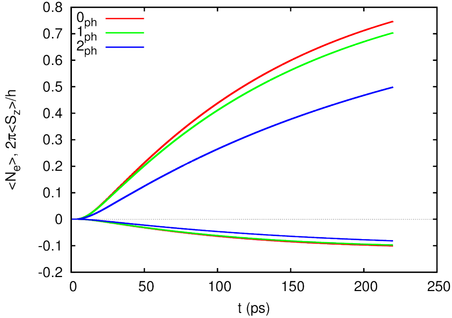
- Spin
- Parallel dots
- $\hbar\Omega_0 = 2.0$ meV
  $\hbar\omega = 1.0$ meV
  $g^{\mathrm{EM}} = 0.2$ meV
  $g = 0.44$
- 36 SES, 120 MES
- 120 MBS

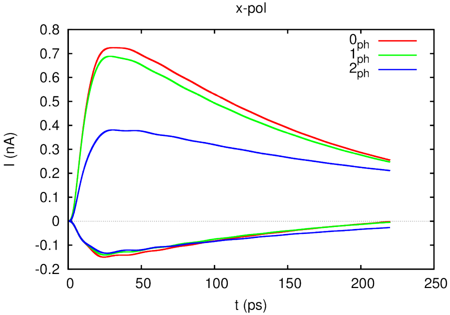


Properties of the closed system



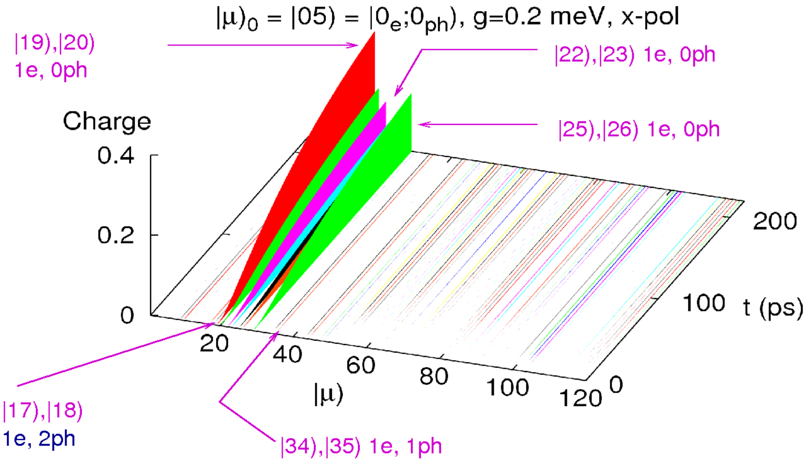
Electron transport, charging empty system



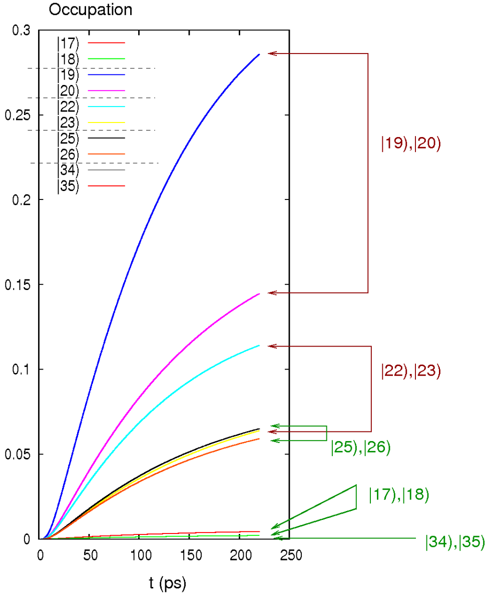


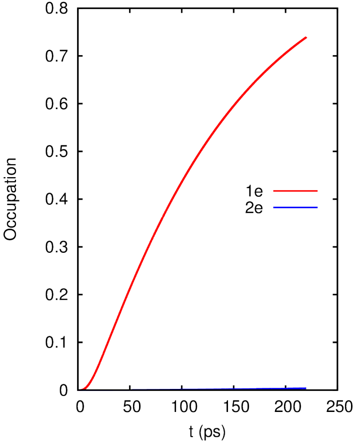
Multi-photon processes

Bias window: |11) --- |21)   **Spin pairs**



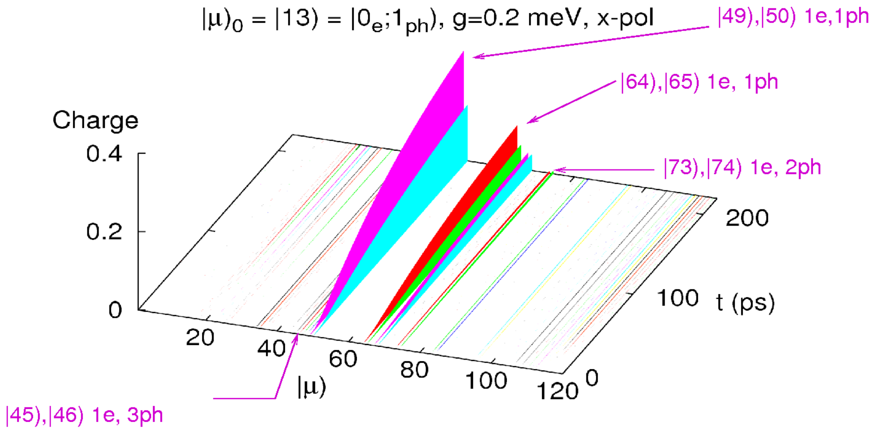
Spin


Occupation
|17)
|18)
|19)
|20)
|22)
|23)
|25)
|26)
|34)
|35)
|19),|20)
|22),|23)
|25),|26)
|17),|18)
|34),|35)
t (ps)

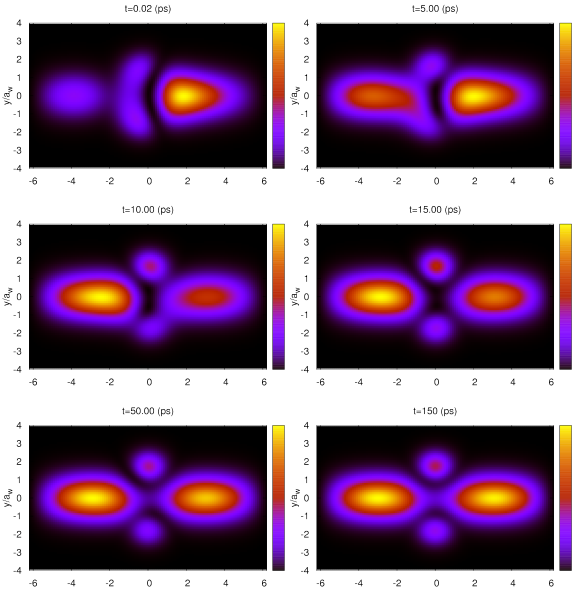

Occupation
1e
2e
t (ps)

Multi-photon processes

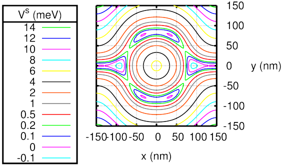
Spin pairs

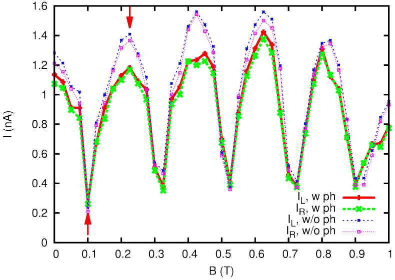


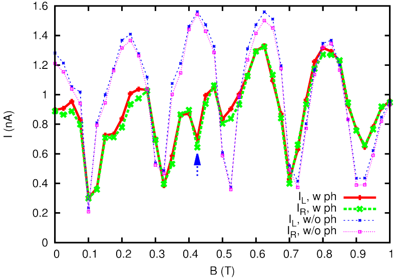
Time-dependent charge



Photon attenuated and assisted transport







Thorsten Arnold, http://arxiv.org/abs/1209.2888

Summary

- Non markovian time-dependent electron transport
- Weak lead-system coupling – strong coupling to a cavity photon mode
- Numerically exact Coulomb and one-photon-mode interaction
- Finite bias, beyond linear response
- Geometrical effects, external homogeneous magnetic field
- Many-body correlations of photons and electrons with spin
- Freedom in choosing initial states
- Parallelization for CPU's, but difficult for GPU's