Time-dependent Green's Functions approach to nuclear reactions

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Encuentros de Física Nuclear 2010

A. Rios *et al.*, arXiv:1009.0215

P. Danielewicz (MSU, NSCL)
B. Barker (MSU, NSCL)

Outline

1. Motivation
2. 1D mean-field dynamics
3. Correlated time evolution
4. Outline

Time matters!

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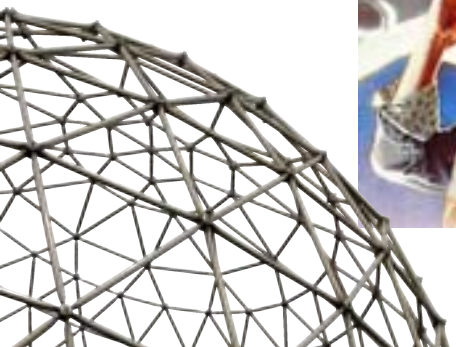
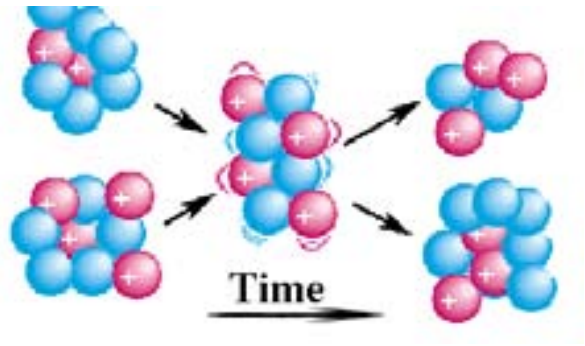
Nuclear reactions are time-dependent processes

- Advancements of time-dependent many-body techniques are needed
  - Central collisions of heavy isotopes $\Rightarrow$ many participants, rearrangement
  - Low-energy fusion reactions $\Rightarrow$ sub-barrier fusion, neck formation
  - Response of finite nuclei $\Rightarrow$ collective phenomena, deexcitation
- Properties of time-dependent Green's function's approach
  - Fully quantal approach
  - Consistent many-body framework
  - Correlations beyond the mean-field approximation





Kadanoff-Baym equations

$$\mathcal{G}^{<}(\mathbf{1}\mathbf{1}') = i\left\langle \Phi_0 \middle| \hat{a}^{\dagger}(\mathbf{1}')\hat{a}(\mathbf{1}) \middle| \Phi_0 \right\rangle \qquad \mathcal{G}^{>}(\mathbf{1}\mathbf{1}') = -i\left\langle \Phi_0 \middle| \hat{a}(\mathbf{1})\hat{a}^{\dagger}(\mathbf{1}') \middle| \Phi_0 \right\rangle$$

$$\left\{ i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} \right\} \mathcal{G}^{\lessgtr}(\mathbf{1}\mathbf{1}') = \int \mathrm{d}\bar{\mathbf{r}}_1 \Sigma_{HF}(\mathbf{1}\bar{\mathbf{1}})\mathcal{G}^{\lessgtr}(\bar{\mathbf{1}}\mathbf{1}') + \int_{t_0}^{t_1} \mathrm{d}\bar{\mathbf{1}} \left[\Sigma^{>}(\mathbf{1}\bar{\mathbf{1}}) - \Sigma^{<}(\mathbf{1}\bar{\mathbf{1}})\right] \mathcal{G}^{\lessgtr}(\bar{\mathbf{1}}\mathbf{1}') - \int_{t_0}^{t_{1'}} \mathrm{d}\bar{\mathbf{1}}\, \Sigma^{\lessgtr}(\mathbf{1}\bar{\mathbf{1}}) \left[\mathcal{G}^{>}(\bar{\mathbf{1}}\mathbf{1}') - \mathcal{G}^{<}(\bar{\mathbf{1}}\mathbf{1}')\right]$$

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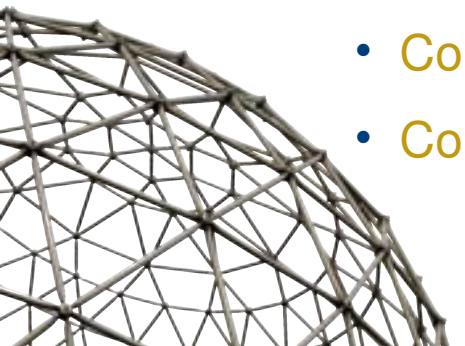
- Evolution of non-equilibrium systems from general principles
- Include correlation and memory effects, via self-energies
- Conservation laws are preserved
- Complicated numerical solution, but very universal framework



Kadanoff & Baym, *Quantum Statistical Mechanics* (1962)

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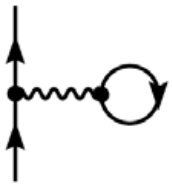
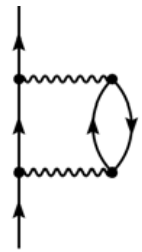
$\Sigma_{HF} \Rightarrow$ 

$\Sigma^{\lessgtr} \Rightarrow$ 

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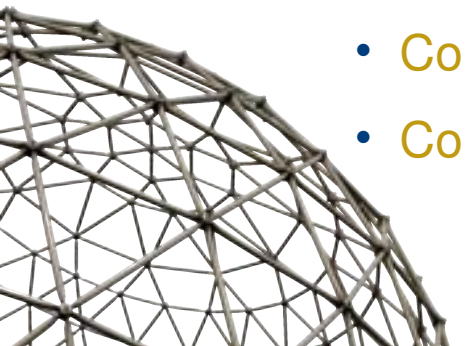

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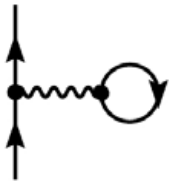
$\Sigma_{HF} \Rightarrow$ 

$$\langle \hat{O} \rangle = -i \lim_{x \to x'} \int \mathrm{d}x\, o(x)\, \mathcal{G}^{<}(x, x'; 0)$$

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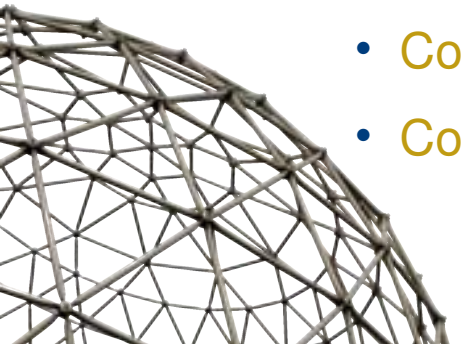
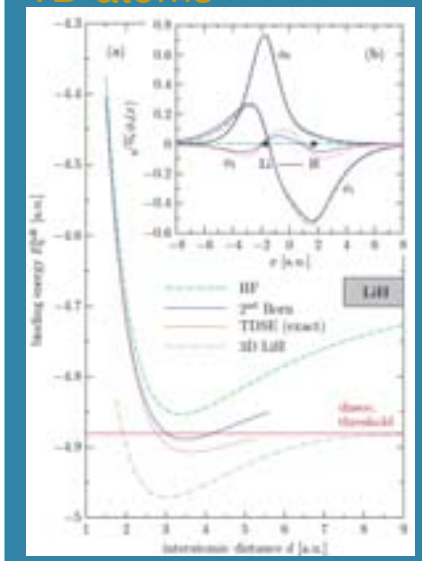


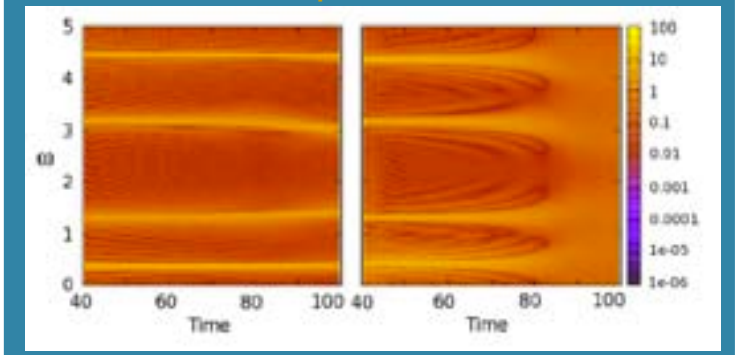
Kadanoff-Baym equations

1D atoms



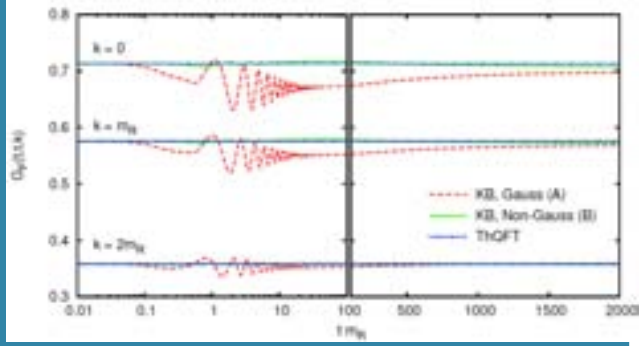
PRA **81**, 022510 (2010)

Quantum transport nanostructures



PRB **80**, 115107 (2009)

Nonequilibrium QFT



PRD **80**, 085011 (2009)

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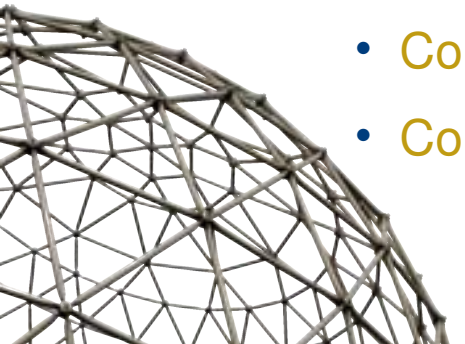
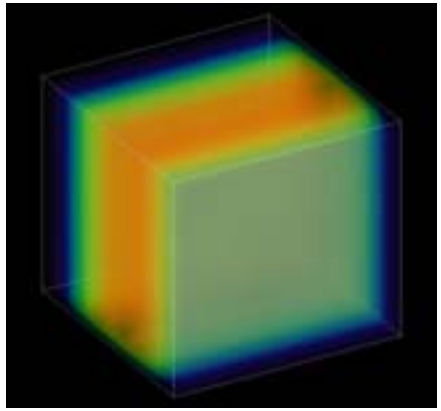


Collisions of 1D slabs



- Frozen & extended y, z coordinates, dynamics in x
- Simple zero-range mean field (1D-3D connection)

$$U(x) = \frac{3}{4} t_0 \, n(x) + \frac{2+\sigma}{16} t_3 \, [n(x)]^{(\sigma+1)}$$

- Attempt to understand nuclear Green's functions
- 1D provide a simple visualization
- Learning before correlations & higher D's

A. Rios *et al.*, arXiv:1009.0215

Collisions of 1D slabs: fusion

$$E_{CM}/A = 0.1\,\mathrm{MeV}$$

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Off-diagonal elements

Importance, elimination & results

1. Systematic analysis of energy dependence
2. Study of origin of off-diagonal elements
3. Assessment of elimination schemes
   - Super-operator erasure of off-diagonal elements
   - Coarse-graining of off-diagonal meshes
4. Impact on time reversibility

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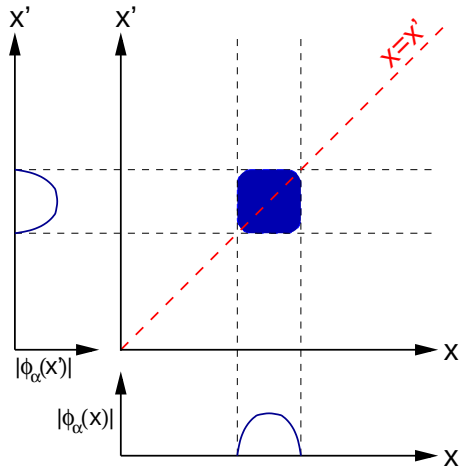

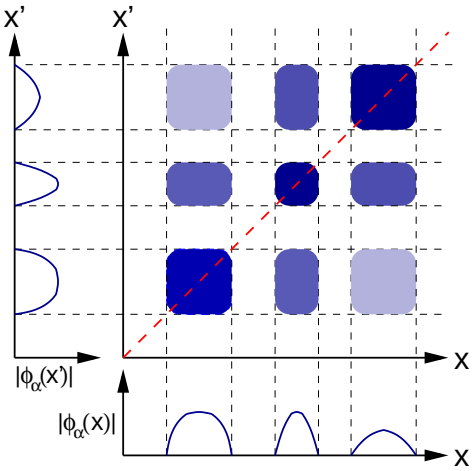

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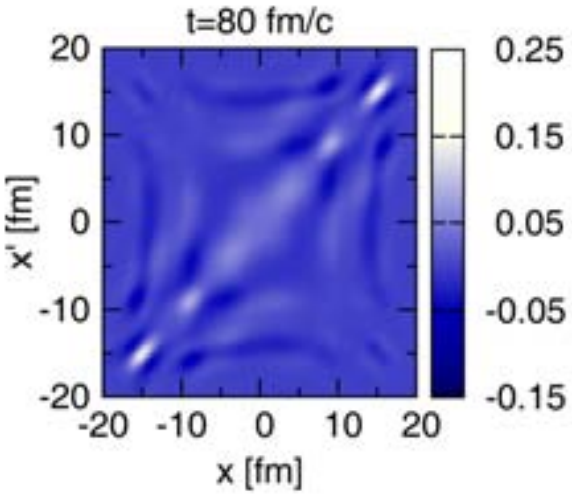

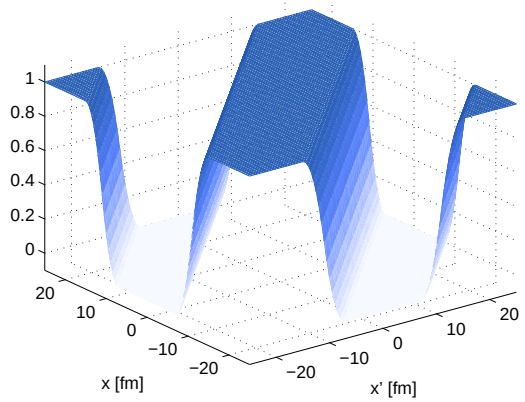

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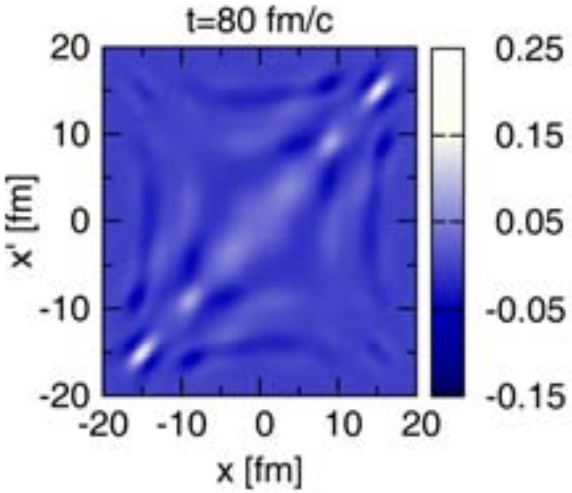

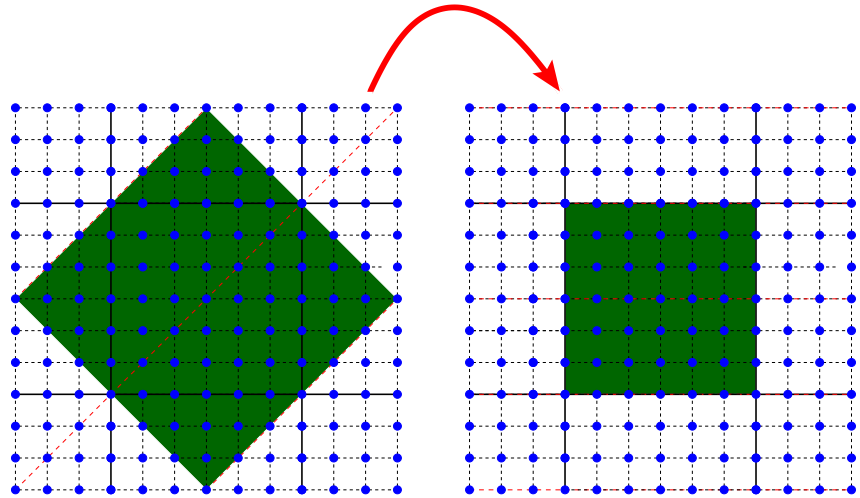

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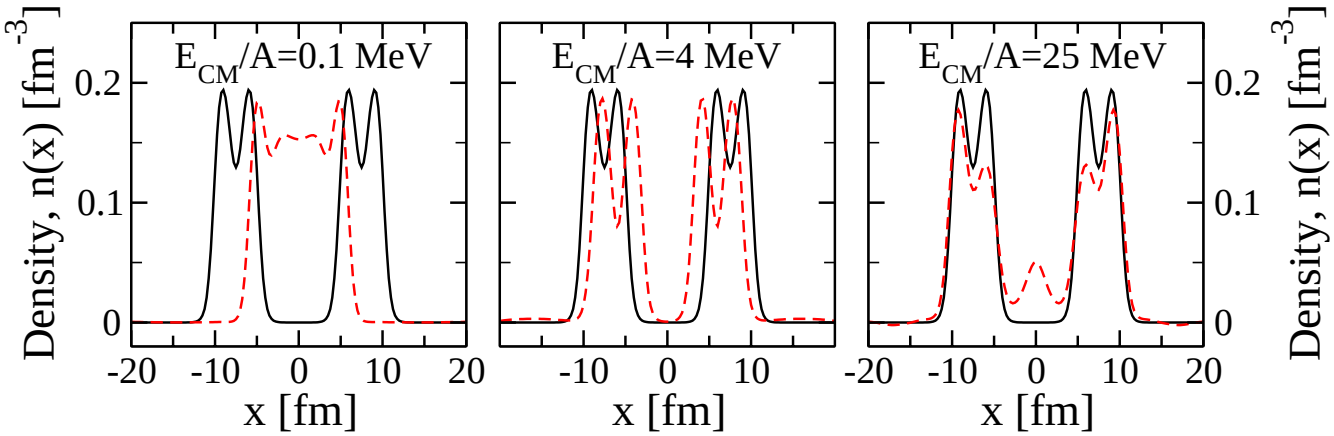

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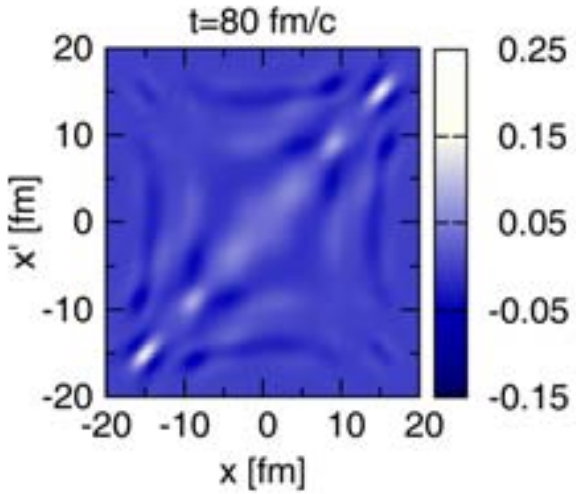
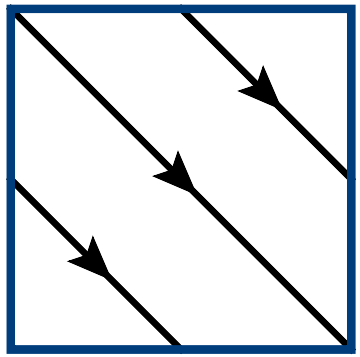
Wigner distribution





- Fourier transform along relative variable (Wigner transform)

$$f_W(x,p) = \int \frac{\mathrm{d}x_r}{2\pi}\, e^{-ipx_r}\, \mathcal{G}^{<}\left(x + \frac{x_r}{2}, x - \frac{x_r}{2}\right)$$

- Simultaneous information on real and momentum space
- Lack of correlations $\Rightarrow$ Wigner valley

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Time evolution beyond the mean-field

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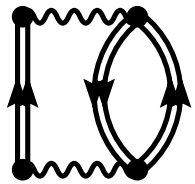
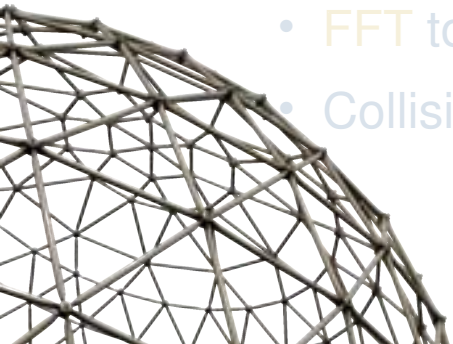


- Direct Born approximation $\Rightarrow$ simplest conserving approximation
- FFT to compute convolution integrals
- Collision integrals $\Rightarrow$ memory effects in 2D $\Rightarrow (t,t')$



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$$\Sigma^{\lessgtr}(p,t;p',t') = \int\frac{\mathrm{d}p_1}{2\pi}\frac{\mathrm{d}p_2}{2\pi}V(p-p_1)V(p'-p_2)\mathcal{G}^{\lessgtr}(p_1,t;p_2,t')\Pi^{\lessgtr}(p-p_1,t;p'-p_2,t')$$

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$$I_1^{>}(p_1,t_1;p_{1'},t_{1'}) = \int_{t_0}^{t_1}\mathrm{d}\bar{t}\int\frac{\mathrm{d}\bar{p}}{2\pi}\left[\Sigma^{>}(p_1,t_1;\bar{p},\bar{t})-\Sigma^{<}(p_1,t_1;\bar{p},\bar{t})\right]\mathcal{G}^{>}(\bar{p},\bar{t};p_{1'},t_{1'})$$
$$-\int_{t_0}^{t_{1'}}\mathrm{d}\bar{t}\int\frac{\mathrm{d}\bar{p}}{2\pi}\Sigma^{>}(p_1,t_1;\bar{p},\bar{t})\left[\mathcal{G}^{<}(\bar{p},\bar{t};p_{1'},t_{1'})-\mathcal{G}^{>}(\bar{p},\bar{t};p_{1'},t_{1'})\right]$$

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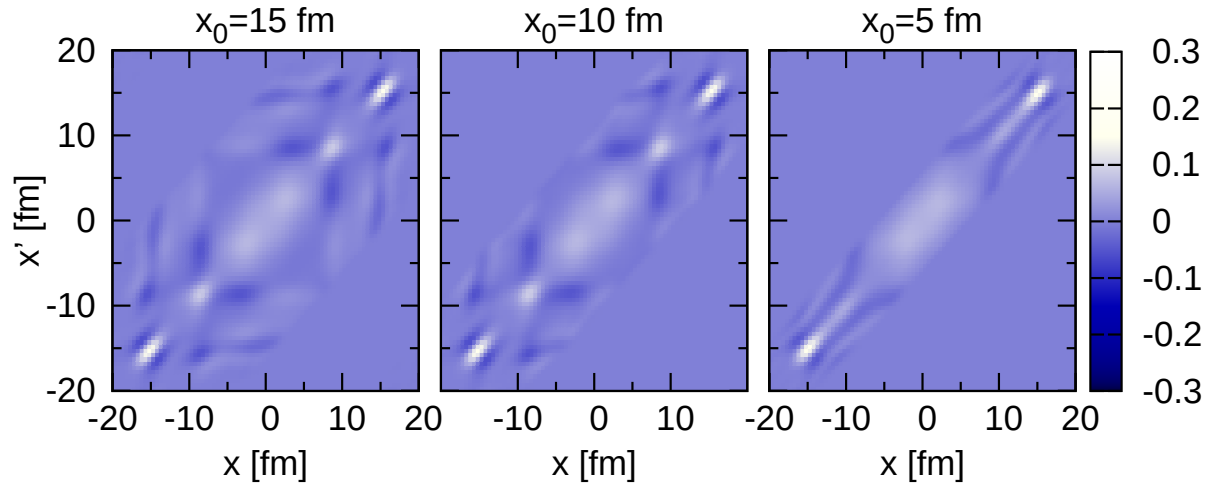
Correlated fermions in a trap

Nuclear Kadanoff-Baym

Potential & challenges



- Mean-field, correlated and off-diagonal elements in 1D $\surd$
- Lessons learned $\Rightarrow$ Progressive understanding of higher D
- Potential for applications in nuclear reactions & structure
- Microscopic understanding of dissipation
- Response for nuclei including collision width
- Multidisciplinary research: from quantum dots to cosmology!

Nuclear Kadanoff-Baym

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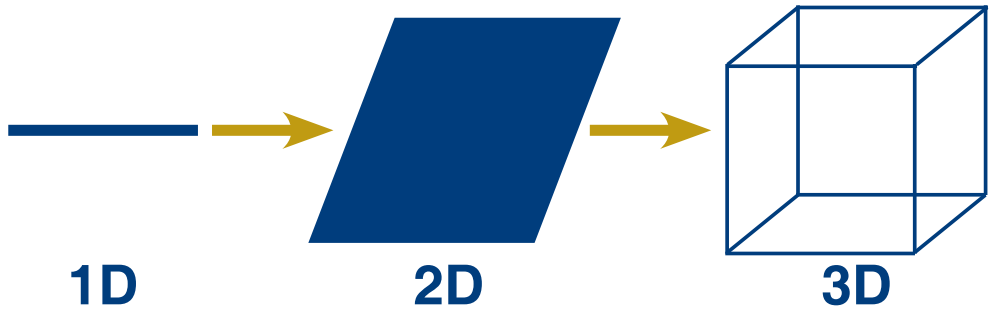

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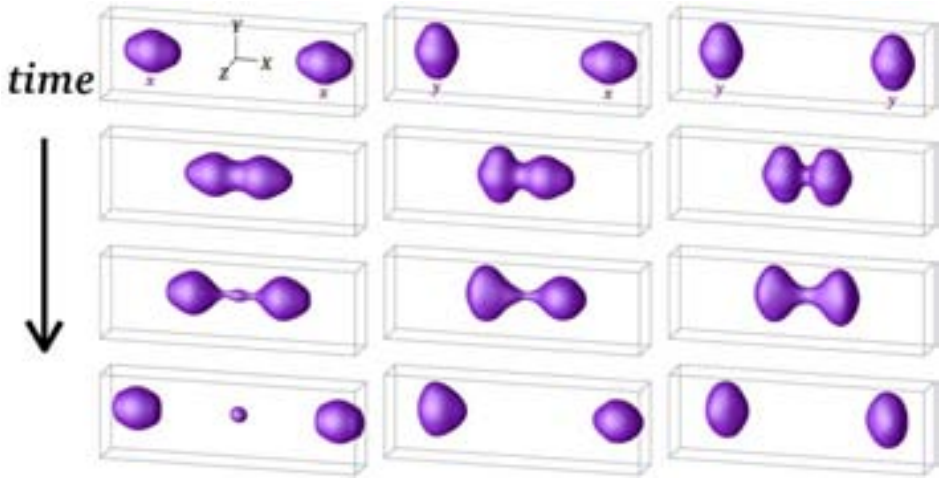

Golabek & Simenel, PRL **103**, 042701 (2009)

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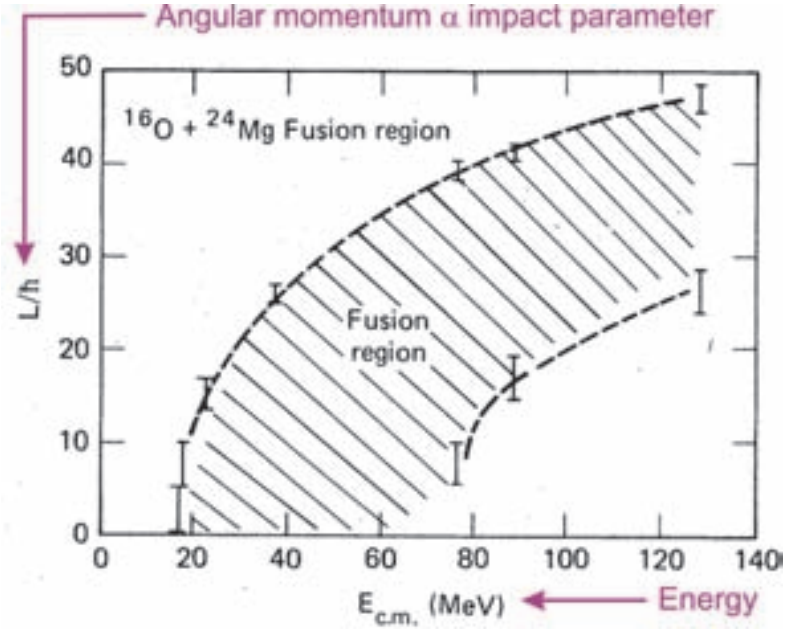

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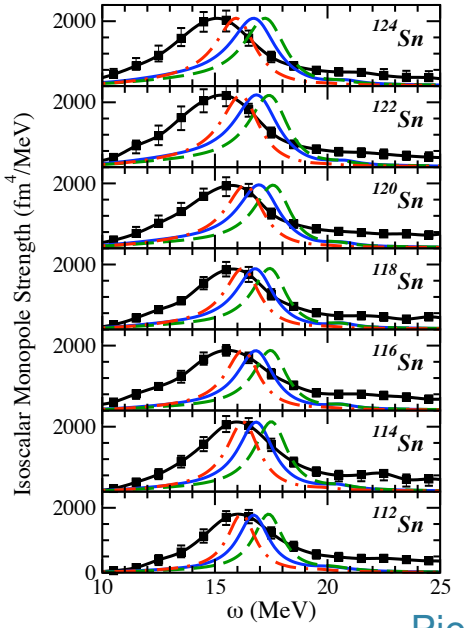
Nuclear Kadanoff-Baym

Potential & challenges



Piekarewicz & Centelles, PRC 79, 054311 (2009)

- Mean-field, correlated and off-diagonal elements in 1D $\surd$
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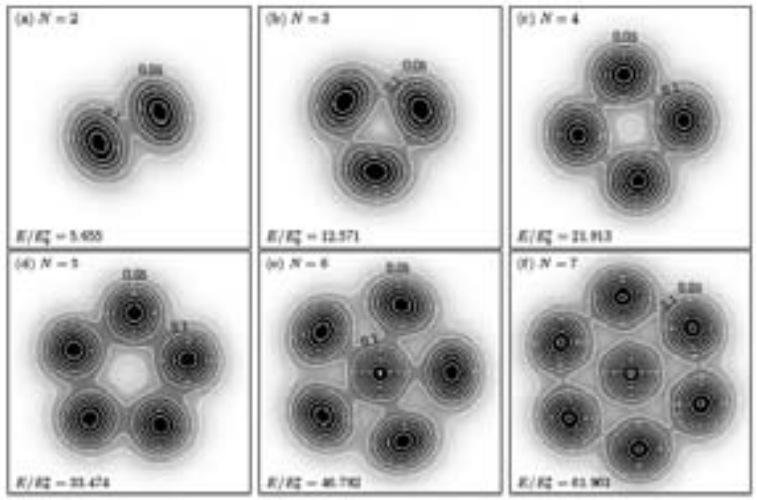

Balzer *et al.*, PRB 79, 245306 (2009)

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Gracias! Gràcies!

A. Rios *et al.*, arXiv:1009.0215

Mean-field evolution: implementation

- The mean-field is time-local
  - $\Sigma_{HF}(\mathbf{11'}) = \delta(t_1 - t_{1'})\,\Sigma_{HF}(x_1, x_{1'})$
  - Only $t_1 = t_{1'} = t$ elements needed: $\mathcal{G}^<(t_1, t_{1'}) \Rightarrow \mathcal{G}^<(t)$
- KB equations reduce to one differential equation

$$i\frac{\partial}{\partial t}\mathcal{G}^<(x,x';t) = \left\{-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + U(x,t)\right\}\mathcal{G}^<(x,x';t)$$
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- Implemented via the Split Operator Method:

$$\text{Small } \Delta t \Rightarrow \mathcal{G}^<(t+\Delta t) \sim e^{-i\left\{\frac{\nabla^2}{2m}+U(x)\right\}\frac{\Delta t}{\hbar}}\mathcal{G}^<(t)e^{+i\left\{\frac{\nabla'^2}{2m}+U(x')\right\}\frac{\Delta t}{\hbar}}$$

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- Calculations in a box & FFT to switch representations

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Mean-field TDGF vs. TDHF

- MF-TDGF and TDHF are numerically equivalent...
- but expressed in different terms!

Time Dependent Green's Functions

$$i\frac{\partial}{\partial t}\mathcal{G}^{<}(x,x';t) = \left\{-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right\}\mathcal{G}^{<}(x,x';t) - \left\{-\frac{1}{2m}\frac{\partial^2}{\partial x'^2} + U(x')\right\}\mathcal{G}^{<}(x,x';t)$$

- 1 equation ... $N_x \times N_x$ matrix
- Testing ground
- Natural extension to correlated case via KB

Time Dependent Hartree-Fock

$$\text{for } \alpha = 1,\ldots,N_\alpha$$

$$i\frac{\partial}{\partial t}\phi_\alpha(x,t) = \left\{-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right\}\phi_\alpha(x,t)$$

$$\text{end}$$

- N_α equations ... vectors of size N_x
- Limited to mean-field!
- Extension needs additional assumptions

Initial state and adiabatic switching

- Initial state should be ground state of the Hamiltonian
  - Mean-field approx. $\Rightarrow$ solve static Hartree-Fock equations
- Possible solution: use adiabatic theorem!

$$H(t) = f(t)H_0 + [1 - f(t)]\, H_1$$

$$f(t) = \begin{cases} 1, & t \to -\infty \\ 0, & t \to t_0 \end{cases}$$

- Advantage: a single code for everything!
- For practical applications:
  - H_0 & H_1 with similar spectra to avoid crossing
  - $H_0 = \frac{1}{2}kx^2$
  - $H_1 = U_{\mathrm{mf}}$
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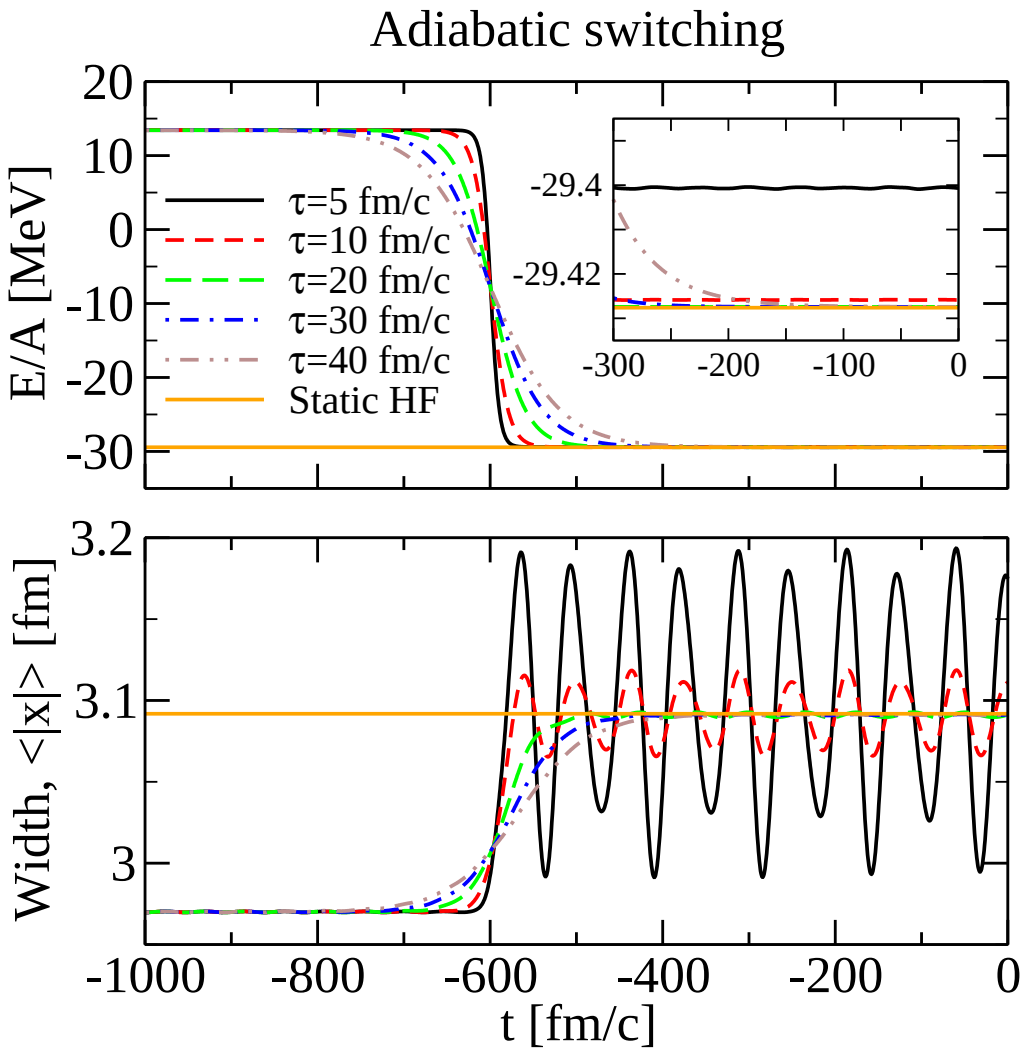
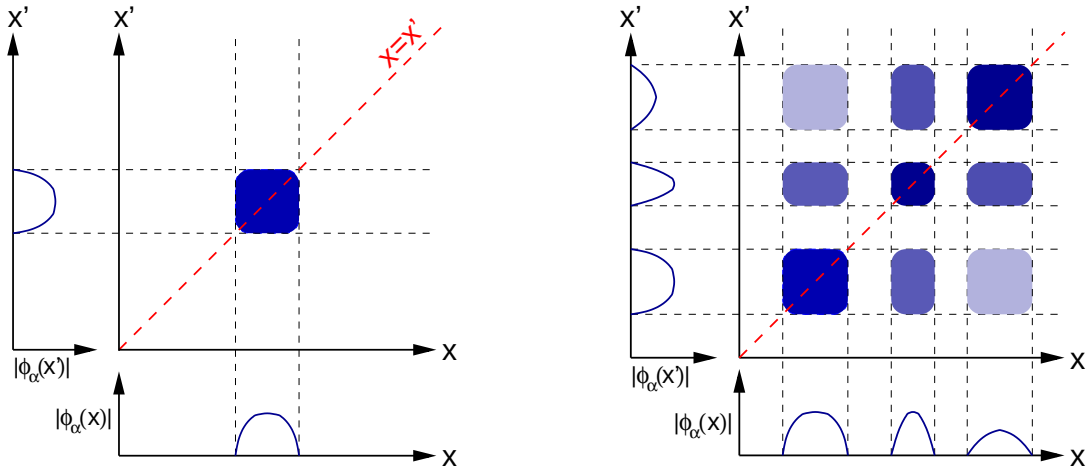
Adiabatic switching & observables



Off-diagonal elements: origin



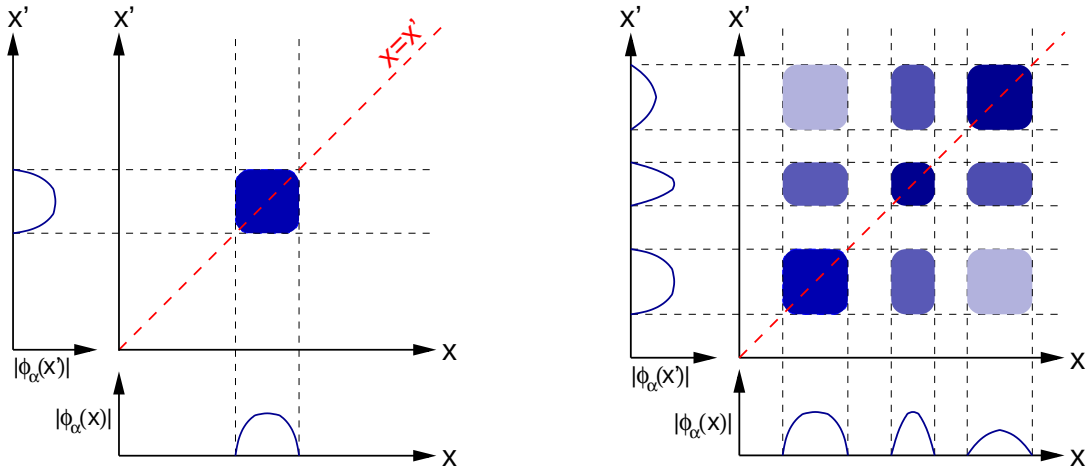
- $\mathcal{G}(x, x')$'s are matrices in x and x'
- Off-diagonal elements describe correlation of single-particle states

$$\mathcal{G}^{<}(x, x') = \sum_{\alpha=0}^{N_\alpha} \phi_\alpha(x)\phi_\alpha^*(x')$$

- Diagonal elements yield physical properties

$$n(x) = \mathcal{G}^{<}(x, x' = x) = \sum_{\alpha=0}^{N_\alpha} n_\alpha |\phi_\alpha(x)|^2 \qquad K = \sum_k \frac{k^2}{2m} \mathcal{G}^{<}(k, k' = k)$$

Off-diagonal elements: importance



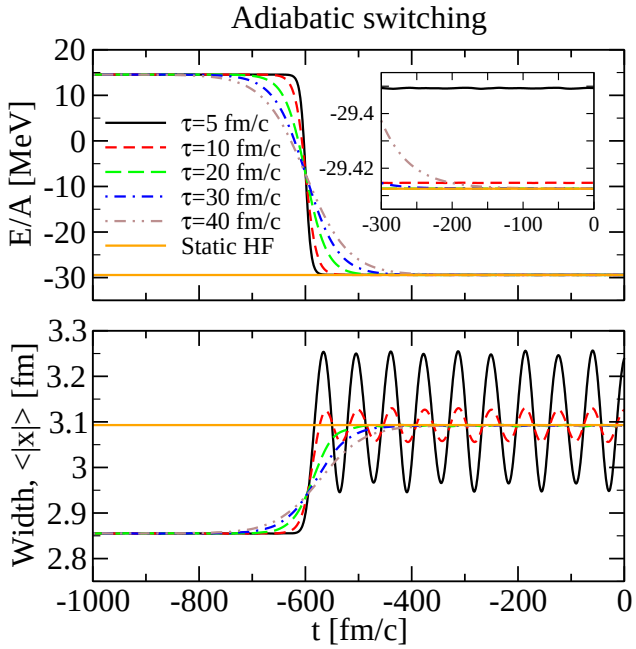
Conceptual issues:

- Should far away sp states be connected in a nuclear reaction?
- Decoherence and dissipation will dominate late time evolution...
- Are $x \neq x'$ elements really necessary for the time-evolution?

Practical issues:

- Green's functions are $N_x^D \times N_x^D \times N_t^2$ matrices: $20^6 \sim 10^8$
- Eliminating off-diagonalities drastically reduces numerical cost

Research program



A. Rios *et al.*, in preparation.

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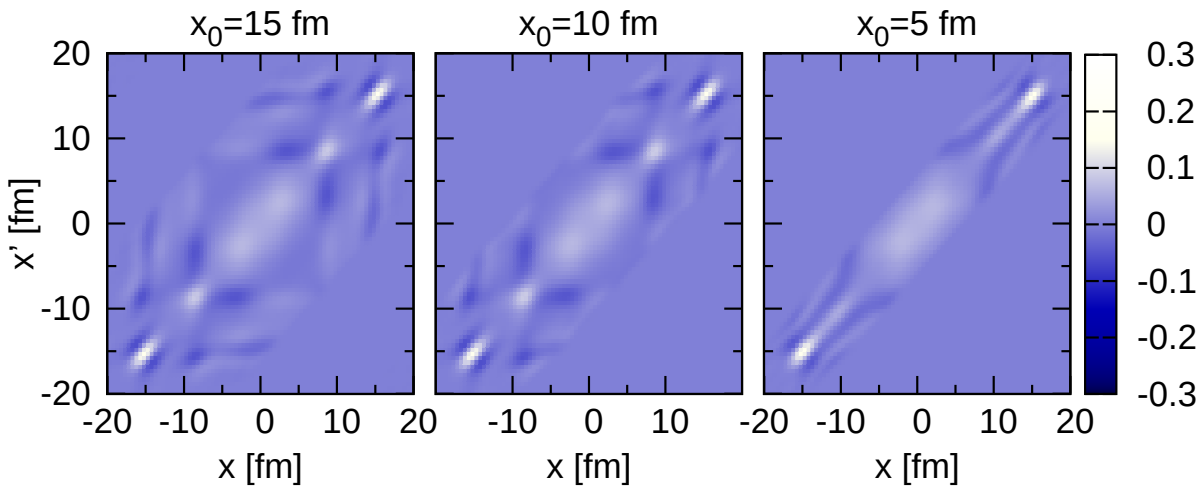

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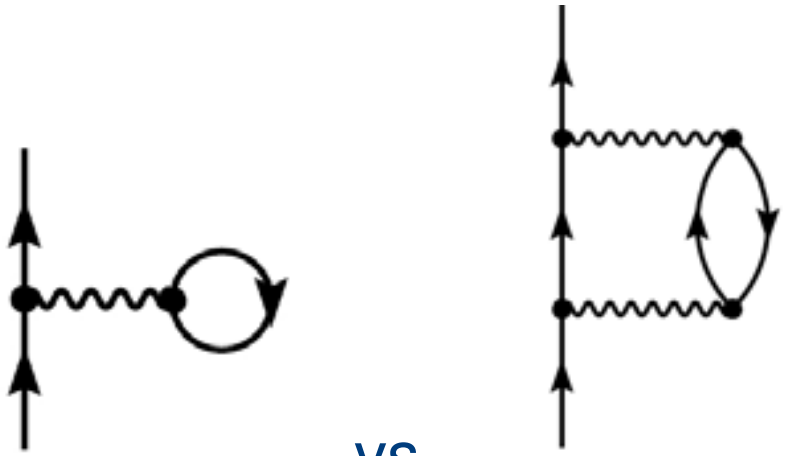

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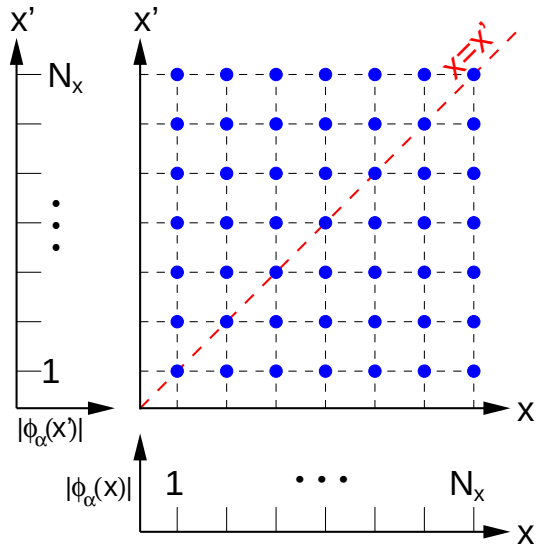
Rotated coordinate frame



- Traditional calculations performed on $N_x \times N_x$ mesh
- Periodic boundary conditions
- Rotated coordinate frame: $x_a = \frac{x+x'}{2}$, $x_r = x' - x$
- Control lengths and meshpoints $\Rightarrow$ $(L_a, N_a) \times (L_r, N_r)$
- Reduce numerical effort by factors of $2 - 10$

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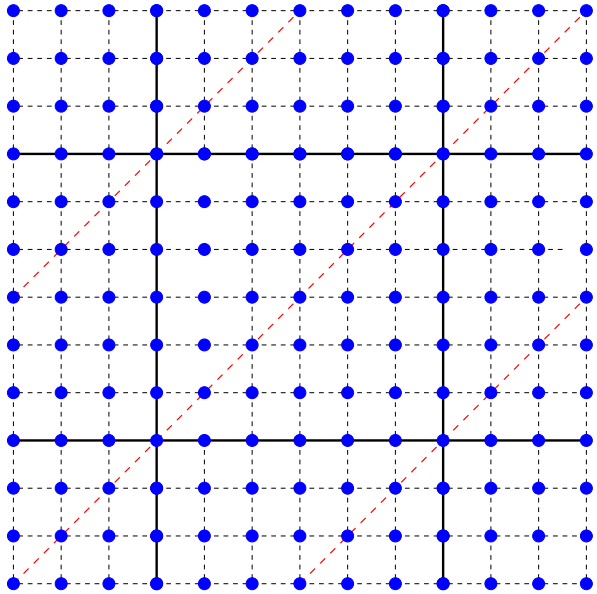

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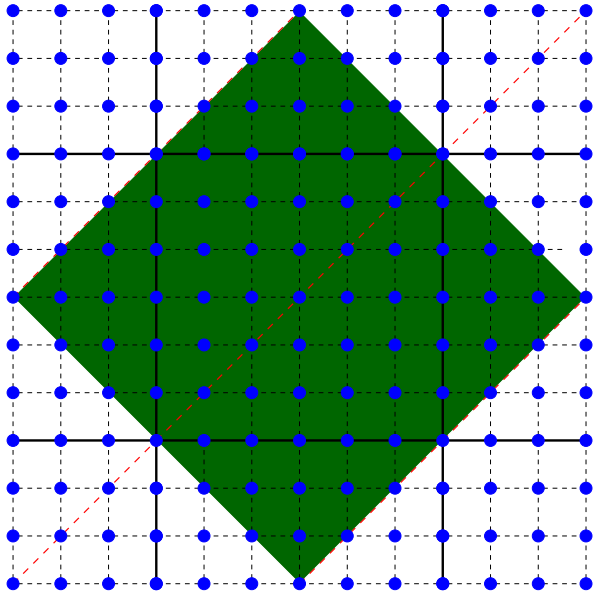

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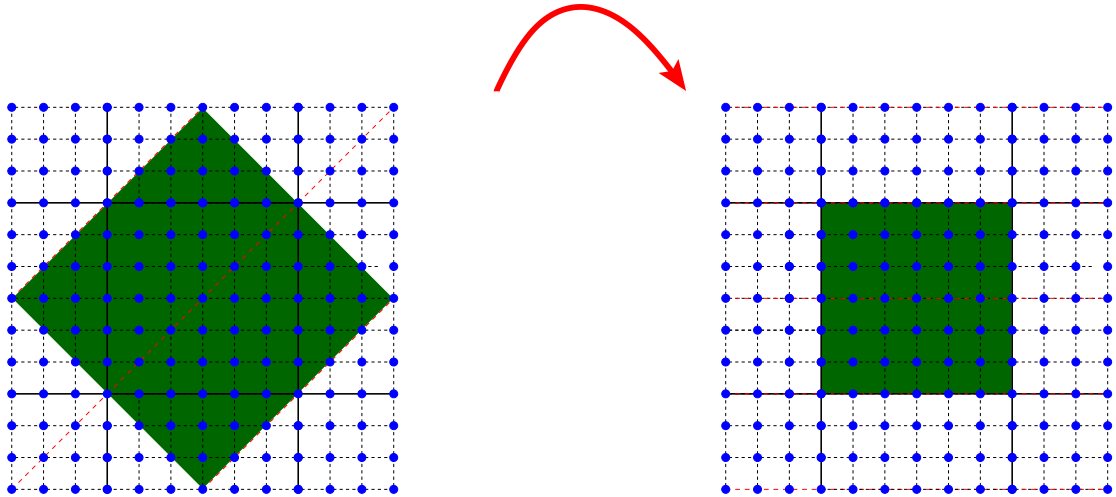

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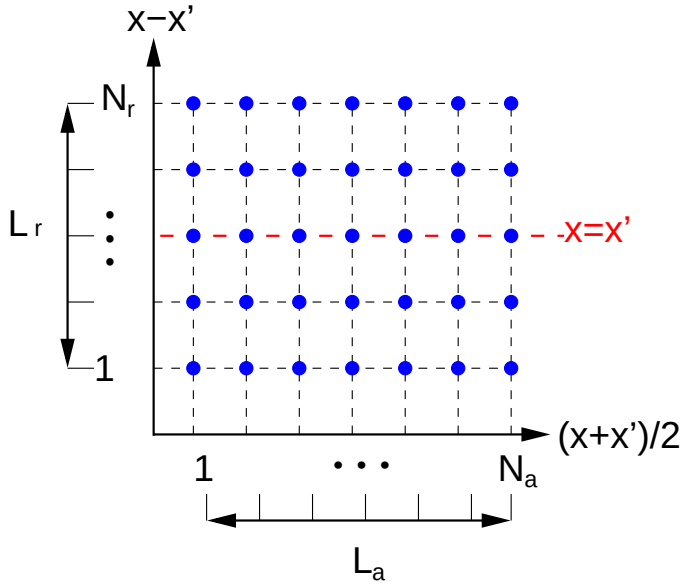

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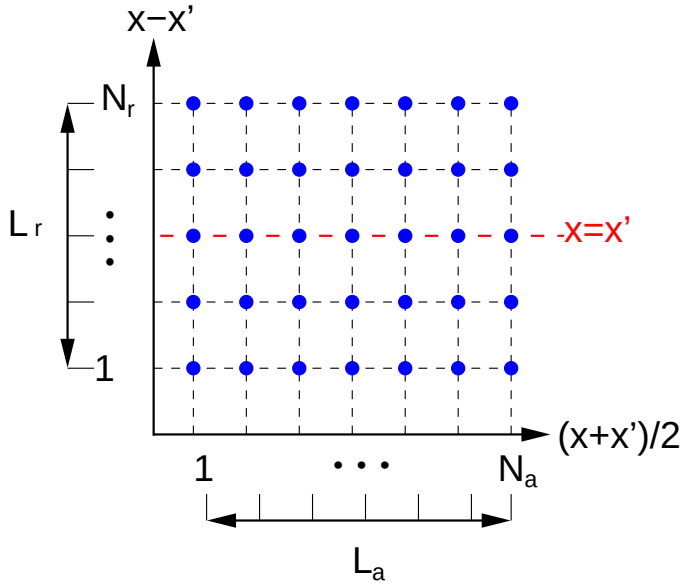

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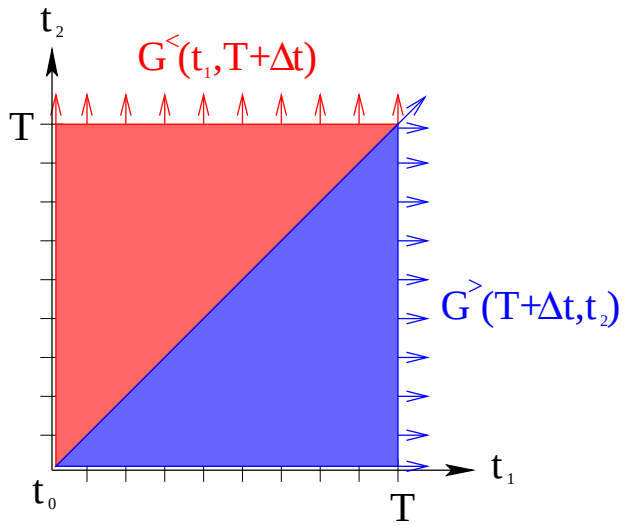
Traditional vs. rotated evolutions

Two time Kadanoff-Baym equations

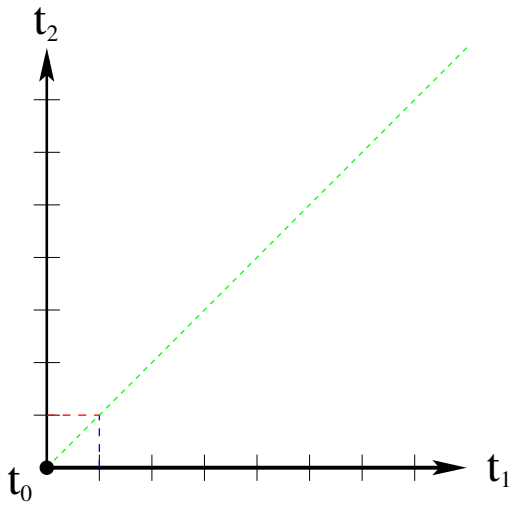
- Need of a strategy to deal with memory & two-times
- Time off-diagonal time elements are present
- Use symmetries $\mathcal{G}^{\lessgtr}(\mathbf{1},\mathbf{2}) = -[\mathcal{G}^{\lessgtr}(\mathbf{2},\mathbf{1})]^*$ to minimize resources
- Self-consistency imposed at every time step



Köhler *et al*, Comp. Phys. Comm. 123, 123 (1999)

Stan, Dahlen, van Leeuwen, Jour. Chem. Phys. 130, 224101 (2009)

Strategy to solve two-time equations



$$\mathcal{G}^<(t_1, T+\Delta t) = e^{i\varepsilon\Delta t}\mathcal{G}^<(t_1, T) - \varepsilon^{-1}\left(1 - e^{i\varepsilon\Delta t}\right)\overline{I_2^<(t_1, T+\Delta t)}$$

$$\mathcal{G}^>(T+\Delta t, t_2) = \mathcal{G}^>(T, t_2)e^{-i\varepsilon\Delta t} - \overline{I_1^>(T+\Delta t, t_2)}\left(1 - e^{-i\varepsilon\Delta t}\right)\varepsilon^{-1}$$

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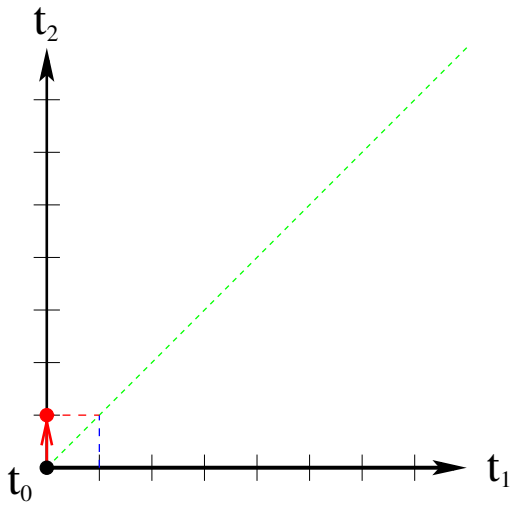
- Each time step involves $2N_t + 1$ operations
- Elimination schemes for time off-diagonal elements?
- Difficult parallelization due to inherent sequential structure

Strategy to solve two-time equations



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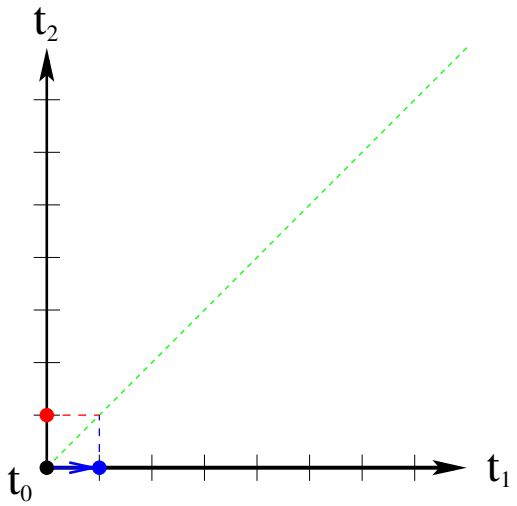

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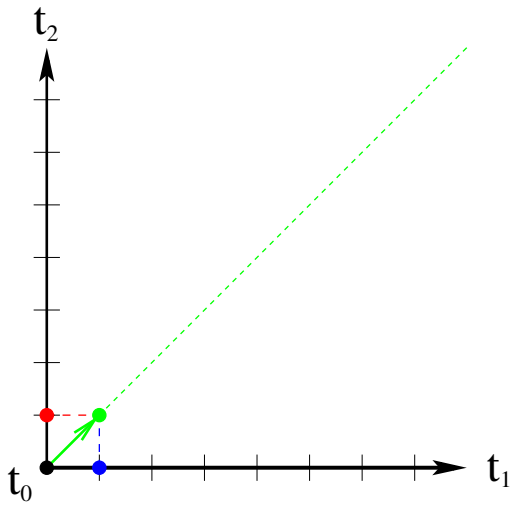

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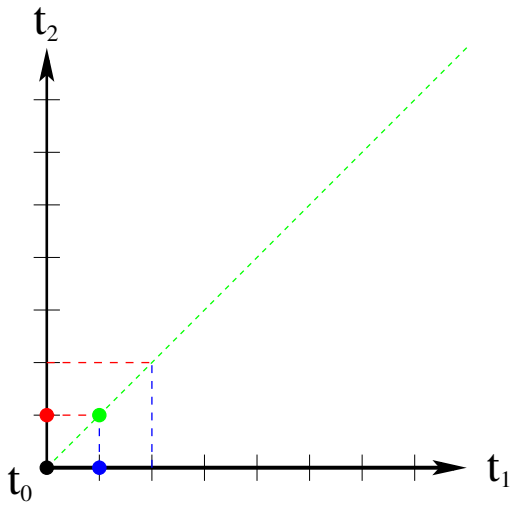

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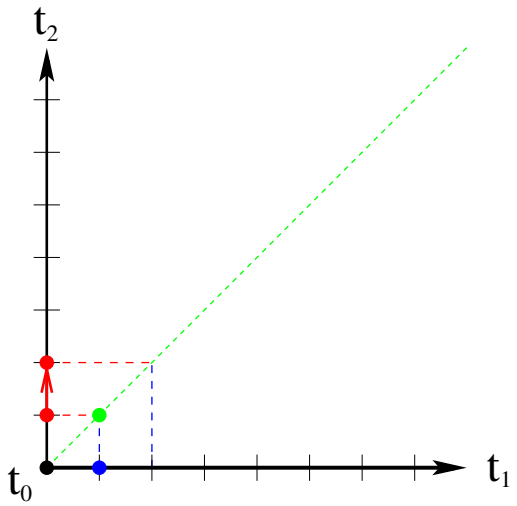
Strategy to solve two-time equations



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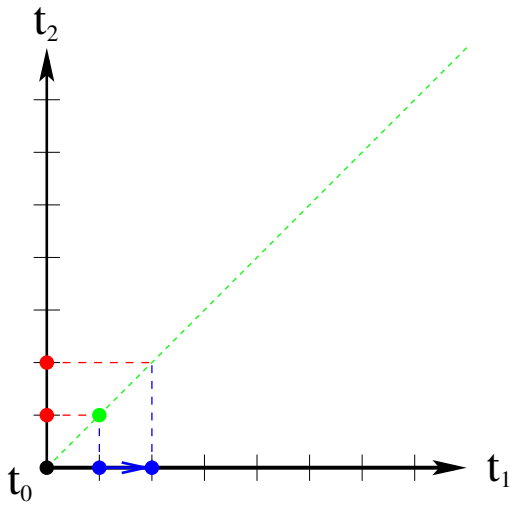

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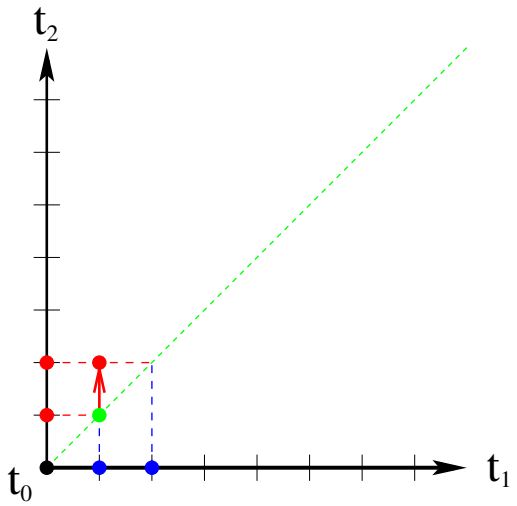

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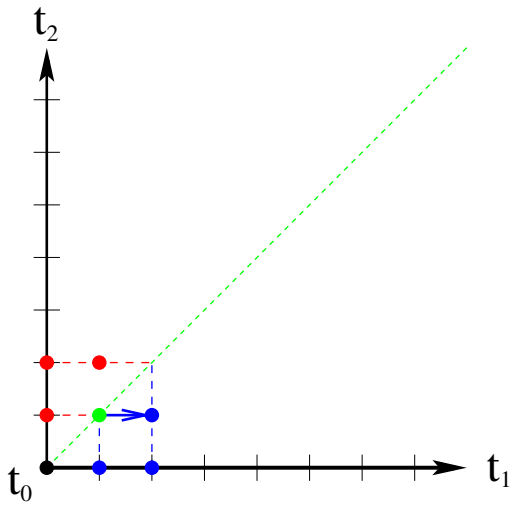

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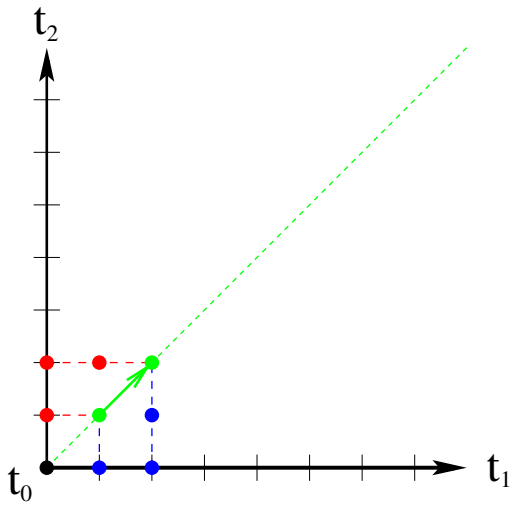

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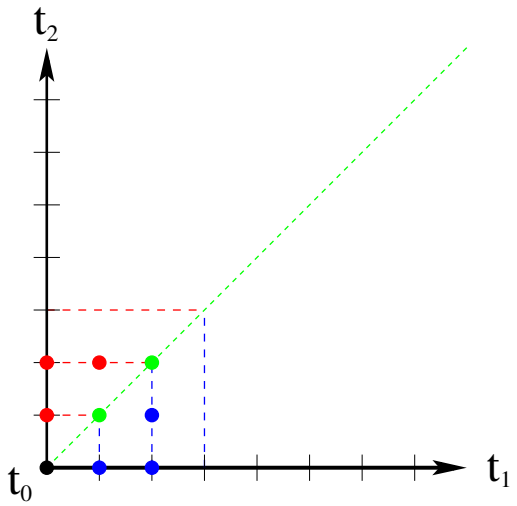

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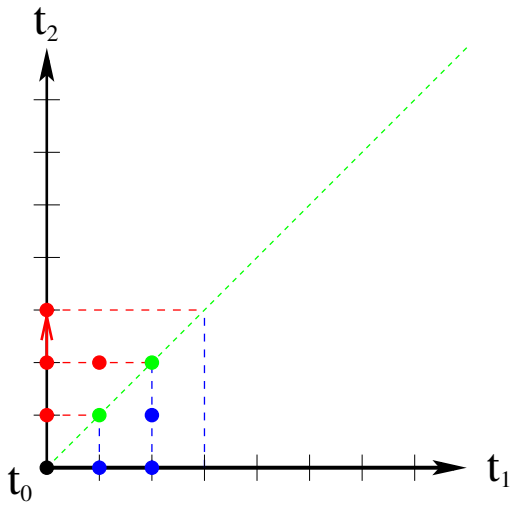

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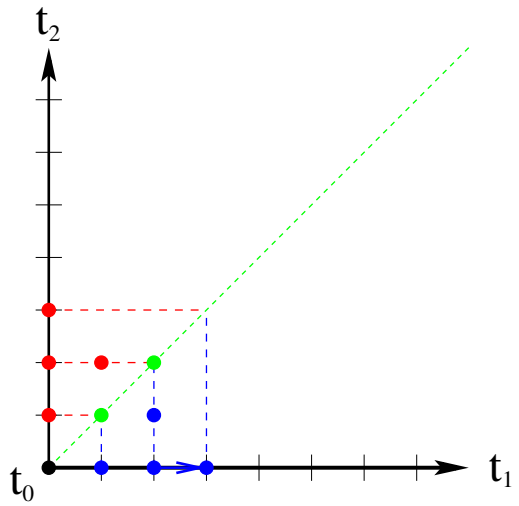

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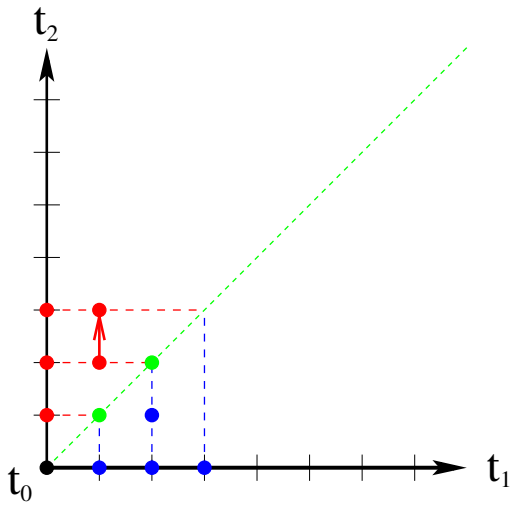

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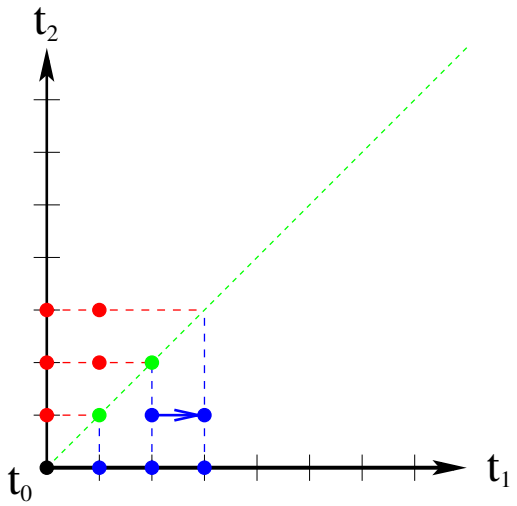

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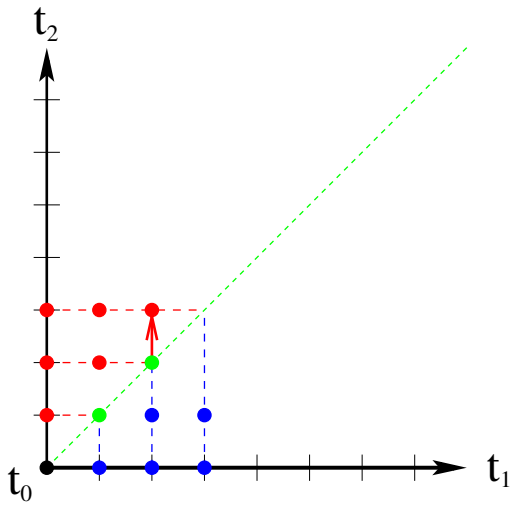

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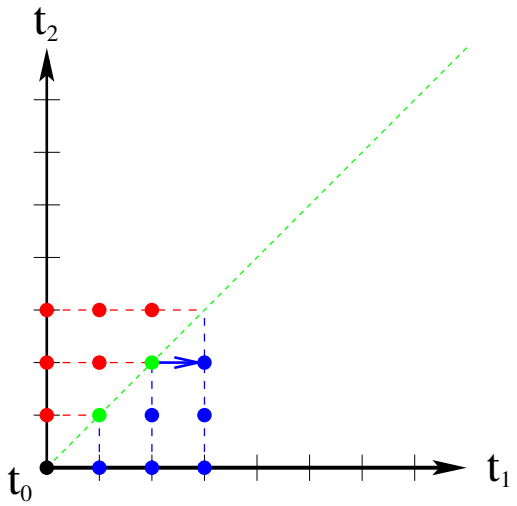

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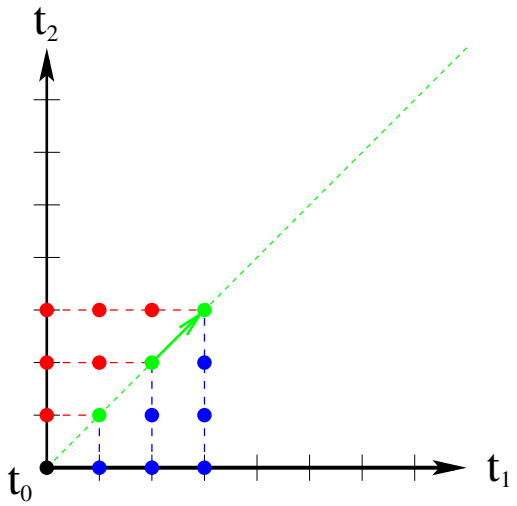

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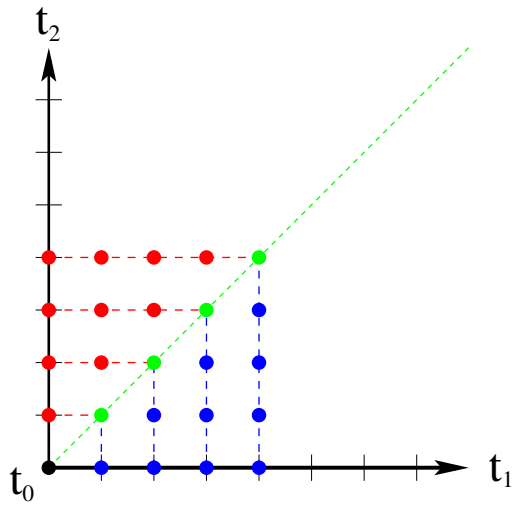

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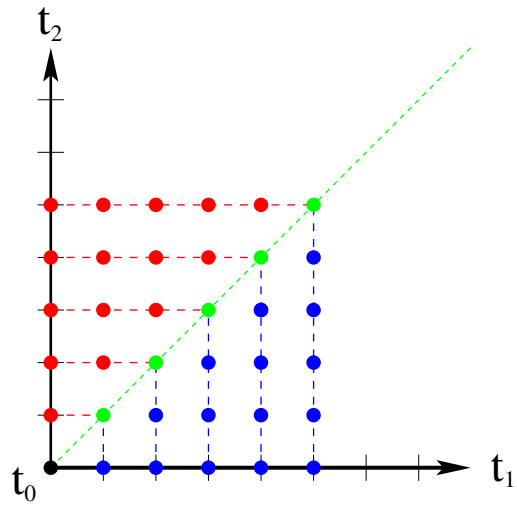

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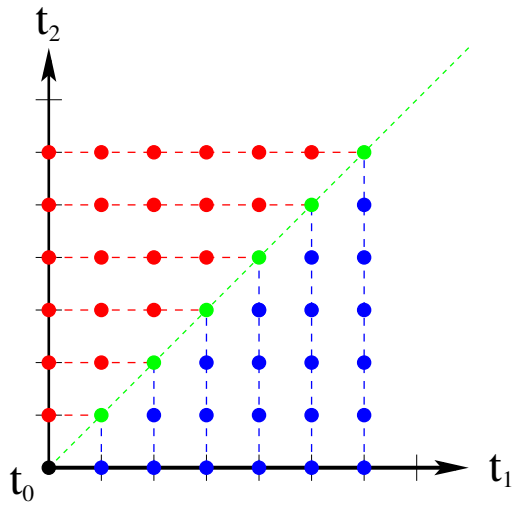

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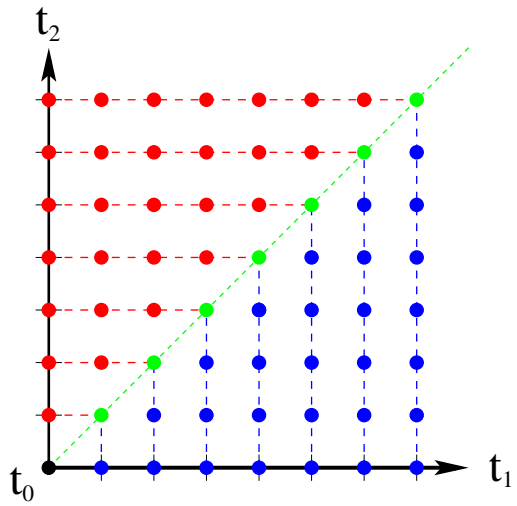

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Nuclear time-dependent correlations

Questions & expectations

- Some experience already gathered for uniform systems

  Danielewicz, Ann. Phys. 152, 239 (1984)

  H. S. Köhler, PRC 51 3232 (1995)

- Expected physical effects
  - Thermalization ($0 < n_\alpha < 1$)
  - Damping of collective modes
- Correlations in the initial state
  - Will a mean-field system evolve to a correlated ground state?
  - Adiabatic switching on of correlations?
  - Imaginary time evolution to get ground states?

- Testing ground calculations: 1D fermions on a HO trap
  - No mean-field, only confining potential
  - Test with mock gaussian NN force
  - Issues with cross section in 1D