Time-dependent Green's Functions method for nuclear reactions

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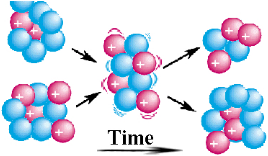
Outline

Time matters!

Nuclear reactions are time-dependent processes!

- Nuclei are self-bound, correlated, many-body systems
- "Scattering" approaches are limited to reaction type & energy...
- Advancements of time-dependent many-body techniques are needed for:
  - Central collisions of heavy isotopes ⇒ many participants, rearrangement
  - Low-energy fusion reactions ⇒ sub-barrier fusion, neck formation
  - Response of finite nuclei ⇒ collective phenomena, deexcitation



TDGF for nuclear reactions

Our goal

Simulate time evolution of correlated nuclear systems in 3D

- Time-Dependent Green's Functions formalism
  - Fully quantal
  - GF's relatively well-understood in static case
  - Beyond mean-field correlations in initial state and in dynamics
  - Microscopic conservation laws are preserved

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
- Complicated numerical solution, but very universal framework
- Already used in other fields.

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

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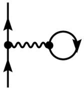
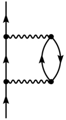
$\Sigma_{HF} \Rightarrow$ 

$\Sigma^{\lessgtr} \Rightarrow$ 

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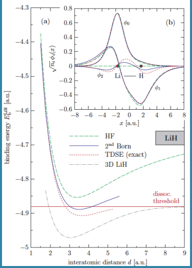
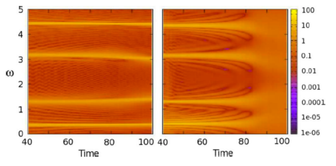
1D molecules



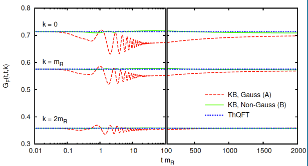
PRA **81**, 022510 (2010)

Quantum transport nanostructures



PRB **80**, 115107 (2009)

Nonequilibrium QFT



PRD **80**, 085011 (2009)

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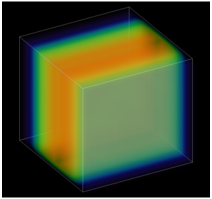
Collisions of 1D slabs



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

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

- Attemp to understand nuclear Green's functions
- 1D provide a simple visualization
- Insight into familiar quantum mechanics problems
- Learning before correlations & higher D's

Mean-field evolution: implementation

- The mean-field is time-local
  - $\Sigma_{HF}(\mathbf{11'}) = \delta\left(t_1 - t_{1'}\right) \Sigma_{HF}(x_1, x_{1'})$
  - 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

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

- Implemented via the Split Operator Method:

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

$$e^{i(\hat{T} + \hat{U})\Delta t} \sim e^{i\frac{\hat{U}}{2}\Delta t} e^{i\hat{T}\Delta t} e^{i\frac{\hat{U}}{2}\Delta t} + O[\Delta t^3]$$

- 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	Time Dependent Hartree-Fock
$i \frac{\partial}{\partial t} \mathcal{G}^{<}(x, x'; t) = \left\{ -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right\} \mathcal{G}^{<}(x, x'; t) - \left\{ -\frac{1}{2m} \frac{\partial^2}{\partial x'^2} + U(x') \right\} \mathcal{G}^{<}(x, x'; t)$	for $\alpha = 1, \ldots, N_\alpha$ $i \frac{\partial}{\partial t} \phi_\alpha(x, t) = \left\{ -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right\} \phi_\alpha(x, t)$ end
• 1 equation ... $N_x \times N_x$ matrix • Testing ground • Natural extension to correlated case via KB	• 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
  - $H_0 = \frac{1}{2}kx^2$
  - $H_1 = U_{\mathrm{mf}}$
  - Adiabatic transient: $f(t) = \frac{1}{1+\mathrm{e}^{(t-\tau_0)/\tau}}, \qquad \tau \to \infty$

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Adiabatic switching: practical examples

$$N_\alpha = 2 \qquad \Longleftrightarrow \qquad A = 8$$

$$U(t) = f(t)\frac{1}{2}kx^2 + [1 - f(t)]\, U_{\mathsf{mf}}(x,t) \qquad \Longleftrightarrow \qquad f(t) = \frac{1}{1 + \mathsf{e}^{(t-\tau_0)/\tau}}$$

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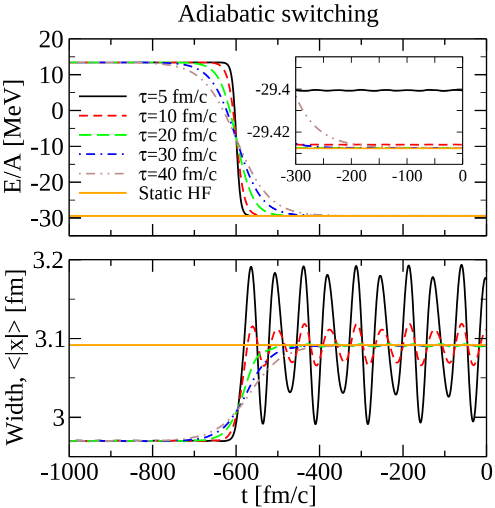
Adiabatic switching & observables



Collisions of 1D slabs: fusion

$$\mathcal{G}^{<}(x,x',P) = e^{iPx}\mathcal{G}^{<}(x,x',P=0)e^{-iPx'}$$

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

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

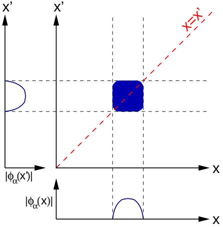
Collisions of 1D slabs: break-up

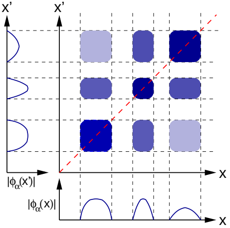
$$\mathcal{G}^<(x, x', P) = e^{iPx}\mathcal{G}^<(x, x', P = 0)e^{-iPx'}$$

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

$$E_{CM}/A = 4\,\mathrm{MeV}$$

Off-diagonal elements: origin





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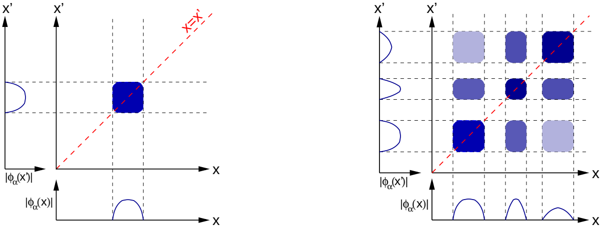
Correlation of single-particle states that are far away

Off-diagonal elements: origin



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Correlation of single-particle states that are far away

Collisions of 1D slabs: multifragment.

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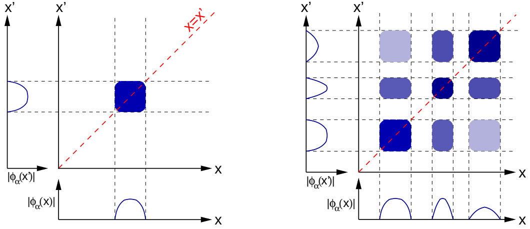
$$\mathcal{G}^{<}(x, x') = \sum_{\alpha < F} \phi_\alpha(x)\phi_\alpha(x')$$

$$E_{CM}/A = 25\,\mathrm{MeV}$$

Off-diagonal elements: origin



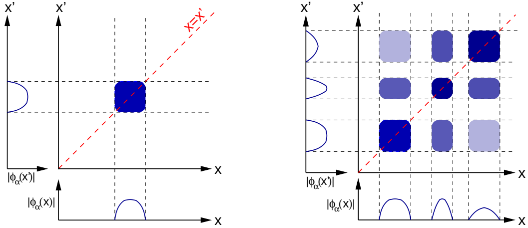
- $\mathcal{G}(x, x')$'s are matrices in x and x'
- Off-diagonal elements describe correlation of single-particle states

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

- 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



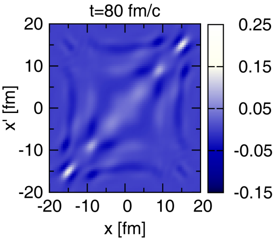
Conceptual issues:

- 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

Off-diagonal elements: cutting procedure



- How can we delete off-diag. without perturbing diagonal evolution?
- Super-operator: act in two positions of $\mathcal{G}^<$ instantaneously
- Use a damping imaginary potential off the diagonal

$$\mathcal{G}^<(x,x',t+\Delta t) \sim e^{i(\varepsilon(x)+iW(x,x'))\Delta t}\mathcal{G}^<(x,x',t)e^{-i(\varepsilon(x')-iW(x,x'))\Delta t}$$

- Properties chosen to preserve: norm, FFT, periodicity, symmetries

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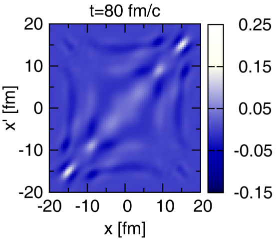

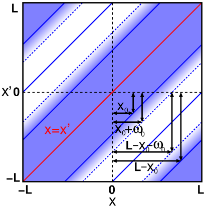

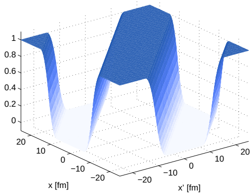

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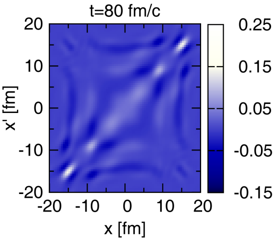

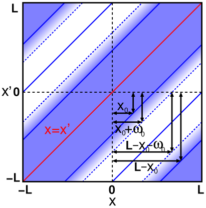

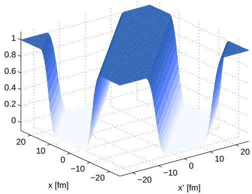

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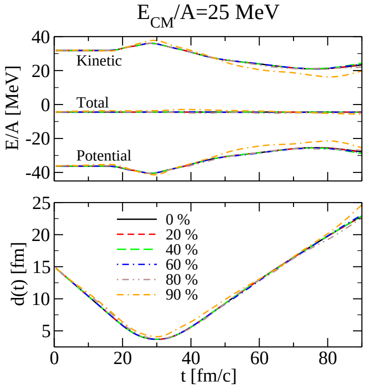
Off-diagonally cut evolution

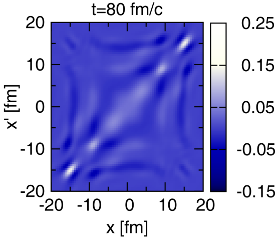
$$E_{CM}/A = 25\,\mathrm{MeV}$$

Cutting off-diagonal elements



- Total energy and different components are unaffected!
- Integrated quantities appear to be cut-independent

Wigner distribution



- Fourier transform along relative variable (Wigner transform)

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

- Simultaneous information on real and momentum space!
- Quantum analog of phase-space density $\rightarrow$ connected to transport

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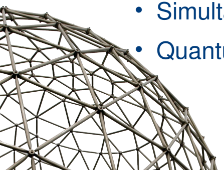
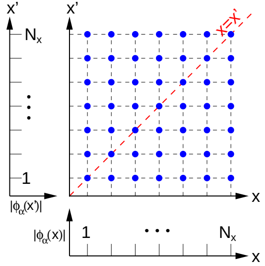


Rotated coordinate frame



- 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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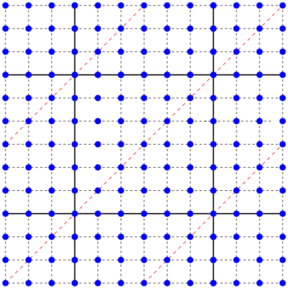

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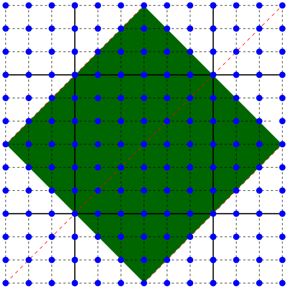

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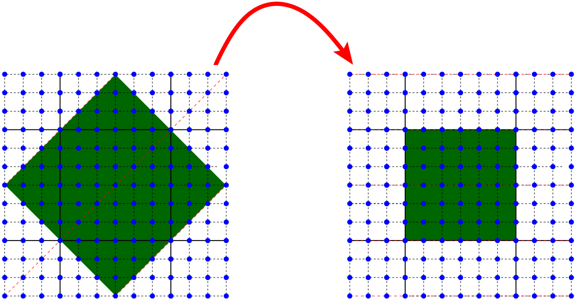

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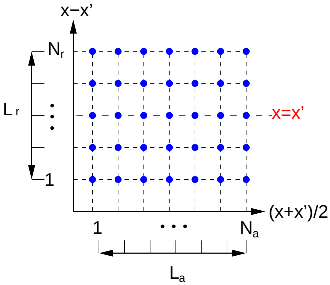

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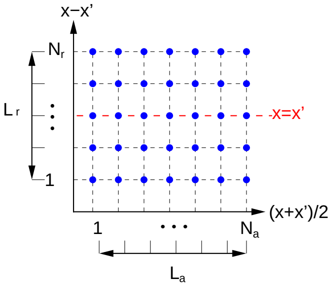

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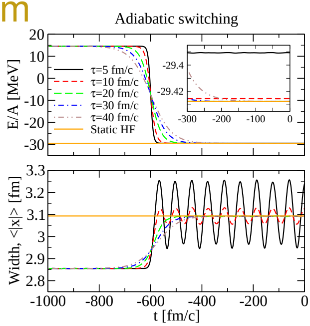
Traditional vs. rotated evolutions

Research program



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

- Used adiabatic theorem to solve mean-field $\surd$
- Full (N_x^2), damped & cut $(N_a \times N_r)$ 1D mean-field evolution $\surd$
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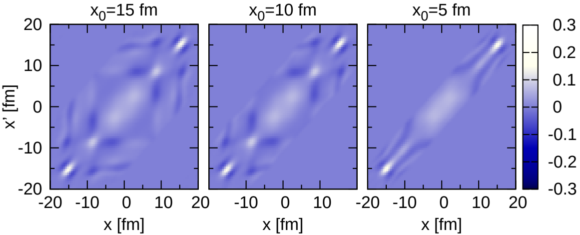
Research program



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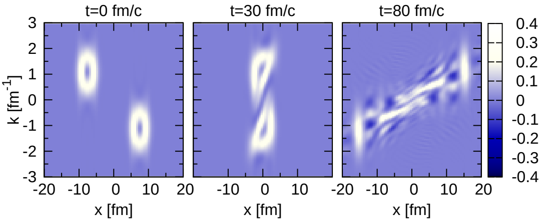

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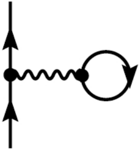
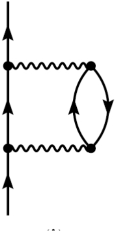


vs.



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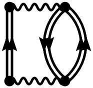
Time evolution beyond the mean-field

$$\left\{-i\frac{\partial}{\partial t_1}-\frac{\nabla_1^2}{2m}-\int \mathrm{d}\bar{\mathbf{r}}_1\Sigma_{HF}(\mathbf{1}\bar{\mathbf{1}})\right\}\mathcal{G}^{\lessgtr}(\mathbf{1}\mathbf{1}')=\underbrace{\int_{t_0}^{t_1}\mathrm{d}\bar{\mathbf{1}}\,\Sigma^R(\mathbf{1}\bar{\mathbf{1}})\mathcal{G}^{\lessgtr}(\bar{\mathbf{1}}\mathbf{1}')+\int_{t_0}^{t_{1'}}\mathrm{d}\bar{\mathbf{1}}\,\Sigma^{\lessgtr}(\mathbf{1}\bar{\mathbf{1}})\mathcal{G}^A(\bar{\mathbf{1}}\mathbf{1}')}_{I_1^{\lessgtr}(\mathbf{1},\mathbf{1}';t_0)}$$



- Direct Born approximation $\Rightarrow$ simplest conserving approximation
- FFT to compute convolution integrals
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- First benchmark calculation to get acquainted with methodology

Time evolution beyond the mean-field

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

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

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

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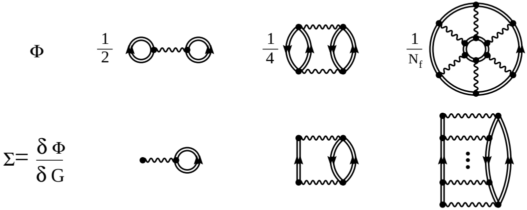

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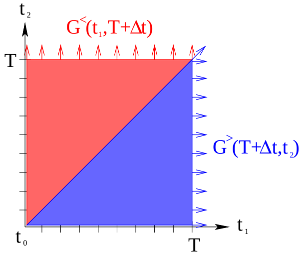
Two time Kadanoff-Baym equations

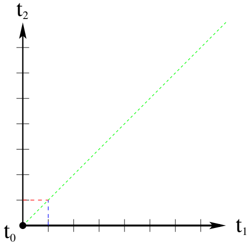
- Need of a strategy to deal with memory & two-times
- Time off-diagonal time elements are present
- Use symmetries $\mathcal{G}^{\lessgtr}(\mathbf{1},\mathbf{2}) = -[\mathcal{G}^{\lessgtr}(\mathbf{2},\mathbf{1})]^*$ to minimize resources
- Self-consistency imposed at every time step



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



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

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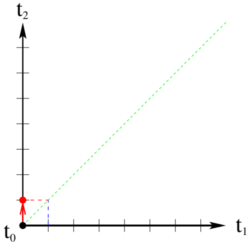
- Each time step involves $2N_t + 1$ operations
- Elimination schemes for time off-diagonal elements?
- Difficult parallelization due to inherent sequential structure

Strategy to solve two-time equations



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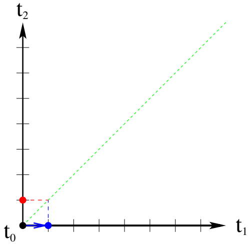

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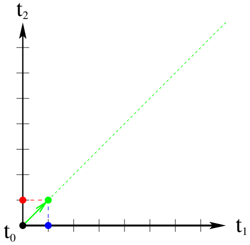

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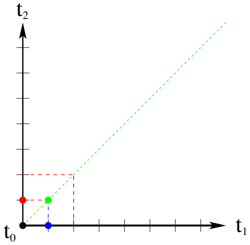

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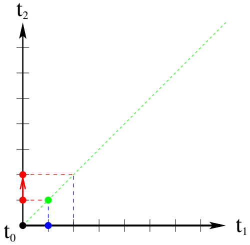

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Strategy to solve two-time equations

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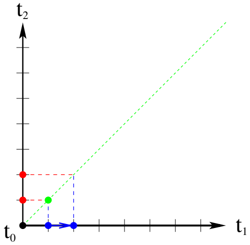

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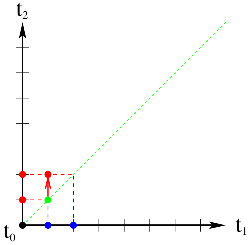

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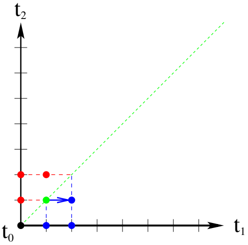

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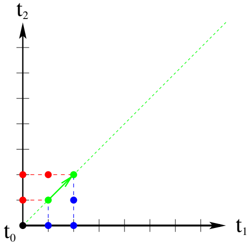

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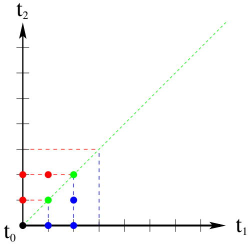
Strategy to solve two-time equations



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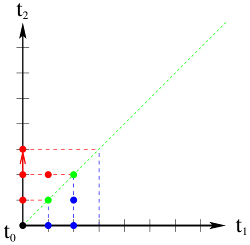

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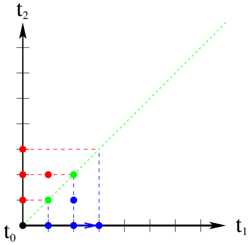

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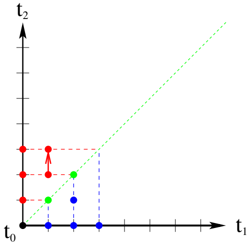

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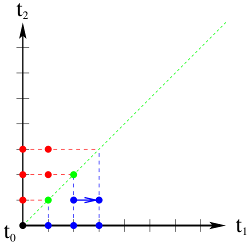

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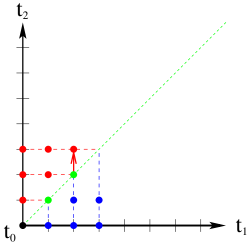

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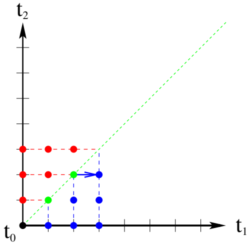

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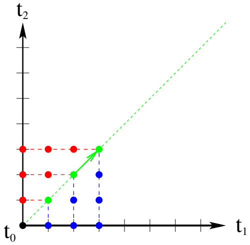

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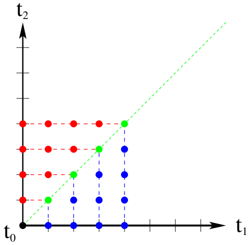

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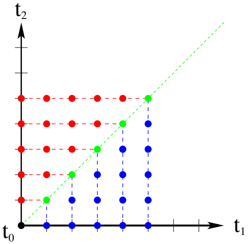

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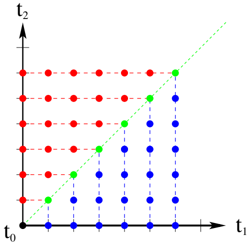

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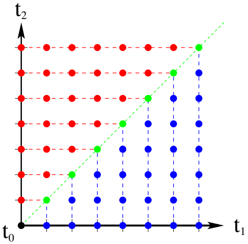

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Nuclear time-dependent correlations

- Some experience already gathered for uniform systems

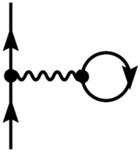
  Danielewicz, Ann. Phys. 152, 239 (1984)

  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

Correlated fermions in a trap

Research program



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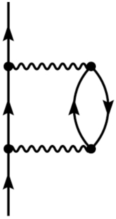

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- Full (N_x^2), damped & cut $(N_a \times N_r)$ 1D mean-field evolution $\surd$
- Identified lack of correlations in Wigner distribution $\surd$
- Full 1D correlated evolution: Born approximation $\sim \surd$
- Lessons learned $\Rightarrow$ Progressive understanding of higher D
- Ultimately: correlated 3D evolution

Research program

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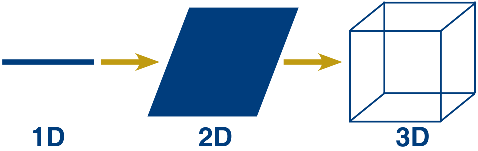

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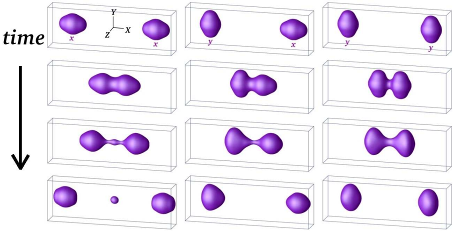

Golabek & Simenel, Phys. Rev. Lett. **103**, 042701 (2009)

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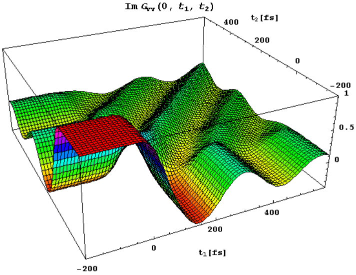
Nuclear Kadanoff-Baym
Potential & challenges



- Potential for applications in nuclear reactions & structure
- Microscopic understanding of dissipation
- Response for nuclei including collision width
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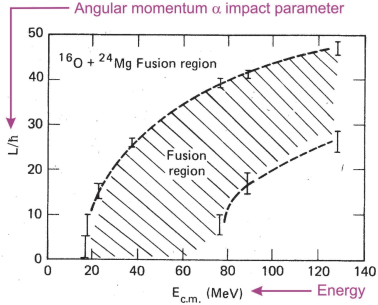

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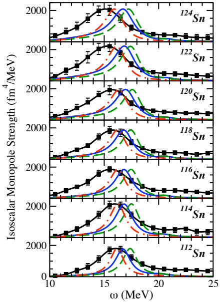

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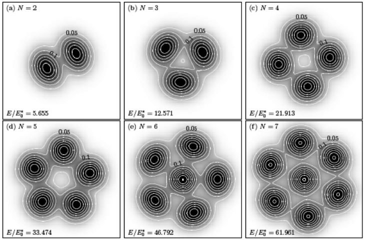

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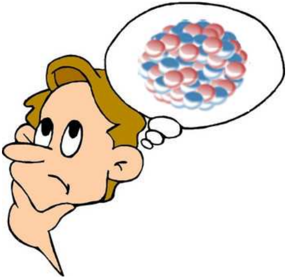

MARIE CURIE ACTIONS PEOPLE Science & Technology Facilities Council