Time-dependent Green's Functions method for nuclear reactions

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Decoherence in Quantum Dynamical Systems
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Collaborators
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Outline

Time matters!

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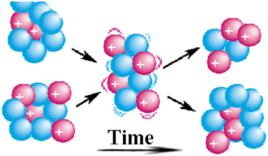
Nuclear reactions are time-dependent processes!

- 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 $\Rightarrow$ many participants, rearrangement
  - Low-energy fusion reactions $\Rightarrow$ sub-barrier fusion, neck formation
  - Response of finite nuclei $\Rightarrow$ 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
  - Conservation laws are preserved
- Peculiarities of our approach:
  - One-body Green's function $\Leftrightarrow$ density matrix
  - Beyond mean-field $\Leftrightarrow$ Memory effects & two times
  - Calculations in box $\Leftrightarrow$ mesh of equidistant N_x points
  - Use of FFT $\Leftrightarrow$ periodic boundary conditions

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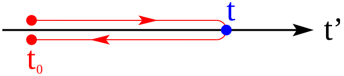
Non-equilibrium Green's functions

Basic formalism: perturbation expansion



$$iG(x_1, t_1; x_{1'}, t_{1'}) = \left\langle T_{\mathcal{C}} \left[a_H(x_1, t_1) a_H^\dagger(x_{1'}, t_{1'}) \right] \right\rangle$$

$$= \left\langle T_{\mathcal{C}} \left[\exp\left(-i \int_{\mathcal{C}} \mathrm{d}t'\, H_I^1(t') \right) a_I(x_1, t_1) a_I^\dagger(x_{1'}, t_{1'}) \right] \right\rangle$$

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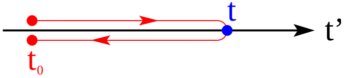

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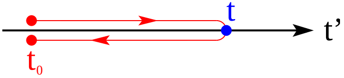
1. Wick decomposition can be performed



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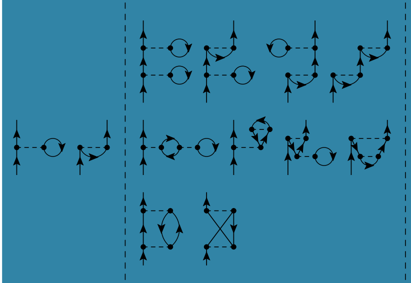
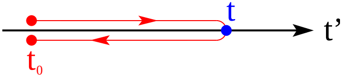
1. Wick decomposition can be performed
2. Feynman diagrams can be defined out of equilibrium!





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1. Wick decomposition can be performed
2. Feynman diagrams can be defined out of equilibrium!
3. Time-dependent observables can be computed

$$\left\langle \hat{O}_H(t) \right\rangle = -i \lim_{x \to x'} \int \mathrm{d}x \, o(x) \, \mathcal{G}^<(x, t; x', t)$$

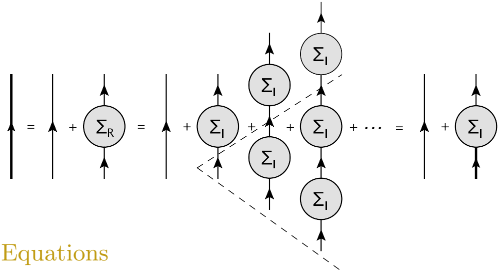
$$\rho(x, x'; t) = -i\mathcal{G}^<(x, t; x', t' = t)$$

$$n(x, t) = -i\mathcal{G}^<(x, t; x' = x, t' = t)$$

$$U(t) = -i\frac{1}{4} \int \frac{\mathrm{d}p}{2\pi} \left\{ i\partial_t - i\partial_{t'} - \frac{p^2}{m} \right\} \mathcal{G}^<(p, t; p, t)$$

Non-equilibrium Green's functions

Basic formalism: conserving approximations



Dyson Equations

$$\left\{ i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} \right\} \mathcal{G}(\mathbf{1},\mathbf{1}') = \delta_{\mathcal{C}}(\mathbf{1},\mathbf{1}') + \int_{\mathcal{C}} \mathrm{d}\mathbf{2}\, \Sigma(\mathbf{1},\mathbf{2})\mathcal{G}(\mathbf{2},\mathbf{1}')$$

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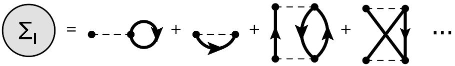

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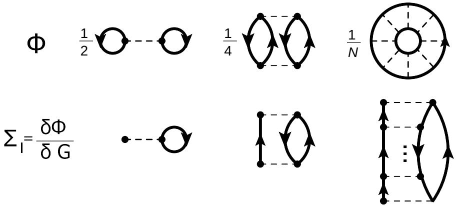

Baym, Phys. Rev. 127, 1391 (1962)

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$$\int_{\mathcal{C}} \mathrm{d}\mathbf{2}\, \Sigma(\mathbf{1},\mathbf{2})\mathcal{G}(\mathbf{2},\mathbf{1}') = i\int \mathrm{d}\mathbf{x}_2\, V(\mathbf{x}_1-\mathbf{x}_2)\mathcal{G}_{II}(\mathbf{1},\mathbf{x}_2,t_1;\mathbf{1}',\mathbf{x}_2,t_1^+)$$

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Kadanoff-Baym equations

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

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

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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.

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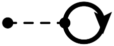
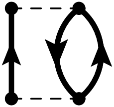
$\Sigma_{HF} \Rightarrow$ 

$\Sigma^{\lessgtr} \Rightarrow$ 

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Kadanoff-Baym equations

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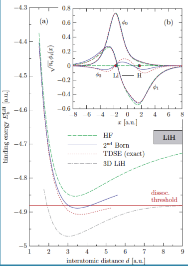
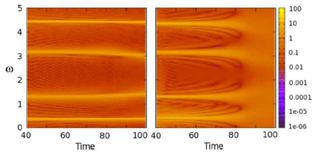
1D atoms



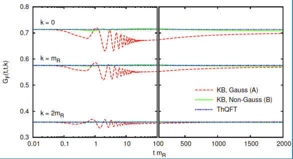
PRA **81**, 022510 (2010)

Quantum transport nanostructures



PRB **80**, 115107 (2009)

Nonequilibrium QFT



PRD **80**, 085011 (2009)

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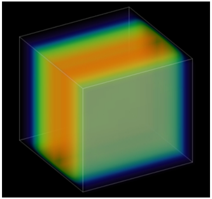
Collisions of 1D slabs



- Frozen & extended y, z coordinates, dynamics in x
- Attemp to understand nuclear Green's functions
- 1D provide a simple visualization
- Insight into familiar quantum mechanics problems
- Simple zero-range mean field (1D-3D connection)

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

Mean-field evolution: implementation

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- 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: $\mathcal{G}^<(t_1, t_{1'}) \Rightarrow \mathcal{G}^<(t)$
- Zero-range mean-field $\Rightarrow$ KB eqs. reduce to 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

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

Time Dependent Green's Functions

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

Time Dependent Hartree-Fock

for $\alpha = 1, \dots, N_\alpha$

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

end

- 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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- For practical applications:
  - H_0 & H_1 with similar spectra to avoid crossing
  - $H_0 = \frac{1}{2} k x^2$
  - $H_1 = U_{\mathrm{mf}}$
  - Adiabatic transient: $f(t) = \frac{1}{1+\mathrm{e}^{(t-\tau_0)/\tau}}, \qquad \tau \to \infty$

Adiabatic switching: practical examples

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

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

Adiabatic switching: practical examples

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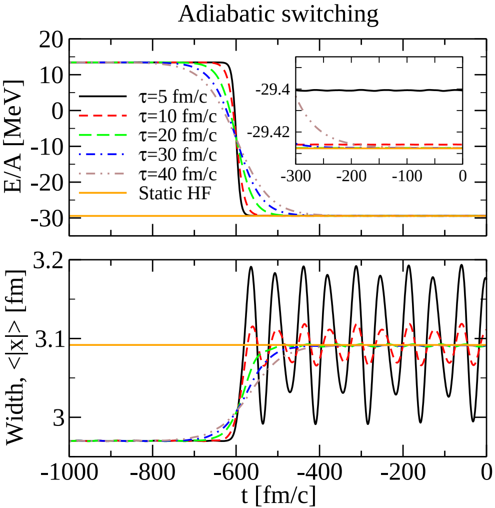
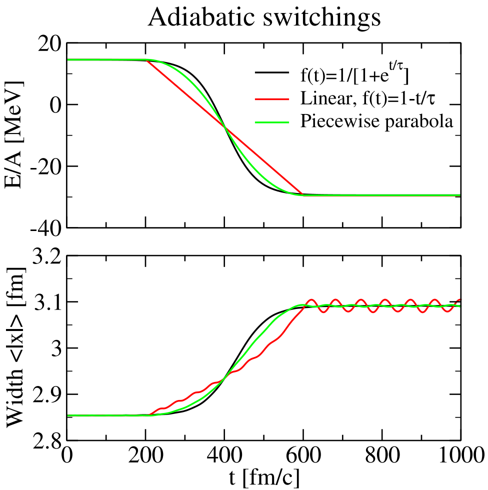
Adiabatic switching & observables



Adiabatic switching & transient function



Collisions of 1D slabs: fusion

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

$$\rho(x, x') = \sum_{\alpha < F} \phi_\alpha(x)\phi_\alpha(x')$$

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

Collisions of 1D slabs: fusion

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

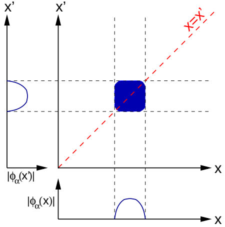
Collisions of 1D slabs: break-up

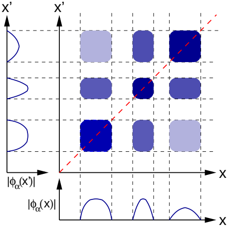
$$\rho(x, x', P) = e^{iPx} \rho(x, x', P = 0) e^{-iPx'}$$

$$\rho(x, x') = \sum_{\alpha < F} \phi_\alpha(x) \phi_\alpha(x')$$

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

Off-diagonal elements: origin

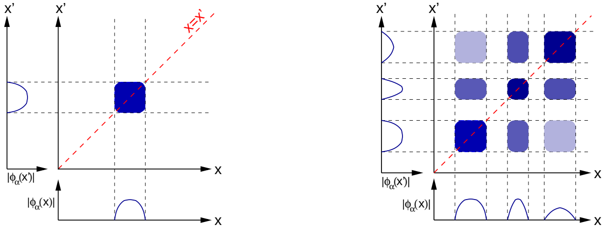




$$\rho(x, x') = \sum_{\alpha<F} \phi_\alpha(x)\phi^*_\alpha(x')$$

Correlation of single-particle states that are far away

Off-diagonal elements: origin



$$\rho(x,x') = \sum_{\alpha<F} \phi_\alpha(x)\phi^*_\alpha(x')$$

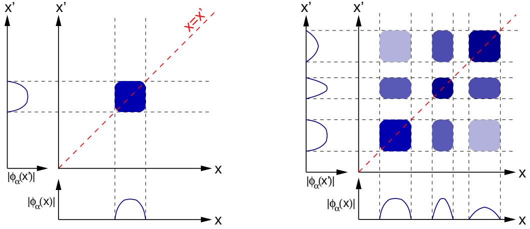
Correlation of single-particle states that are far away

Collisions of 1D slabs: multifragment.

$$\rho(x, x', P) = e^{iPx}\rho(x, x', P = 0)e^{-iPx'}$$
$$\rho(x, x') = \sum_{\alpha<F} \phi_\alpha(x)\phi_\alpha(x')$$

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

Off-diagonal elements: origin



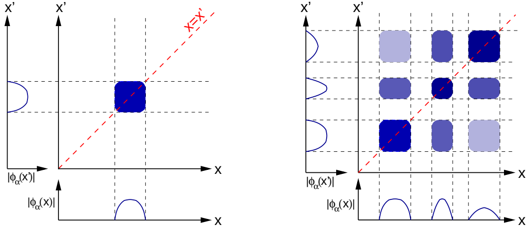
- Off-diagonal elements describe correlation of single-particle states

$$\rho(x,x') = \sum_{\alpha=0}^{N_\alpha} \phi_\alpha(x)\phi^*_\alpha(x')$$

- Diagonal elements yield physical properties

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

Off-diagonal elements: importance



Conceptual issues:

- Should far away sp states be connected in a nuclear reaction?
- Decoherence and dissipation might 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

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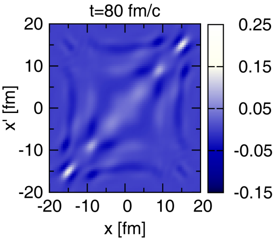
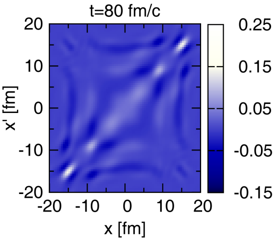


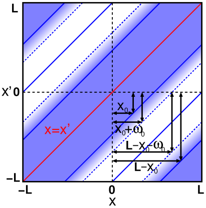
- How can we delete off-diag. without perturbing diagonal evolution?
- Super-operator: act in two positions of $\mathcal{G}^<$ instantaneously
- Use a damping imaginary potential off the diagonal

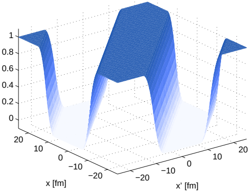
$$\mathcal{G}^<(x,x',t+\Delta t) \sim e^{i(\varepsilon(x)+iW(x,x'))\Delta t}\mathcal{G}^<(x,x',t)e^{-i(\varepsilon(x')-iW(x,x'))\Delta t}$$

- Properties chosen to preserve: norm, FFT, periodicity, symmetries
- *Ad hoc* decoherence ⇒ How large unphysical effects?

Off-diagonal elements: cutting procedure







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Off-diagonal elements: cutting procedure

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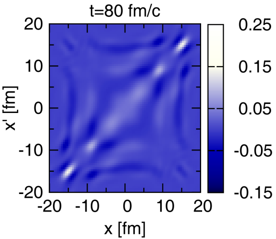

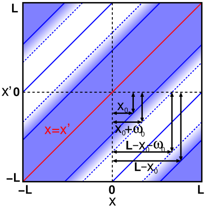

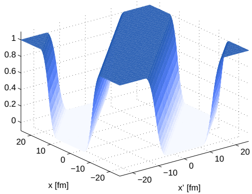

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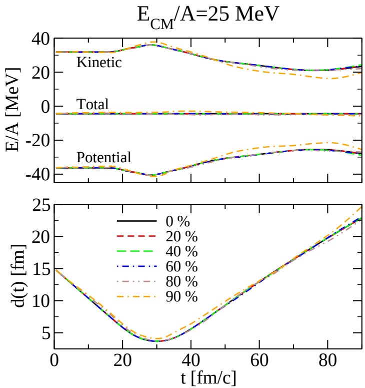
- *Ad hoc* decoherence $\Rightarrow$ How large unphysical effects?

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

Consequences of cuts: irreversibility

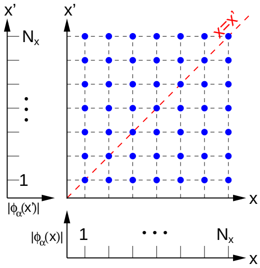
What processes are sensitive to cuts?

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

Uncut evolution, forward & backwards

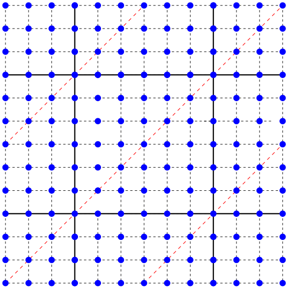
Cut evolution forward $|x - x'| < 10$ fm, uncut backwards

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 $2 - 10$

Rotated coordinate frame



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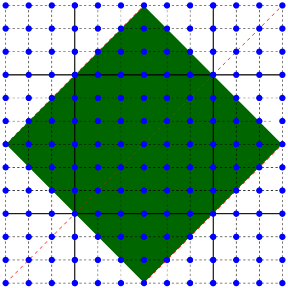

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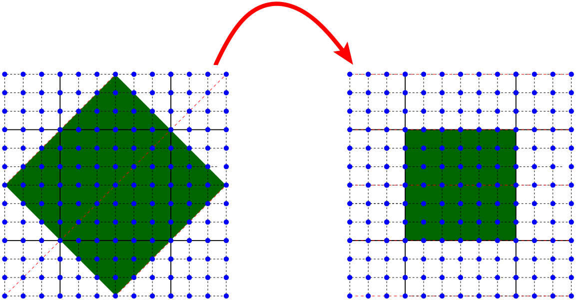

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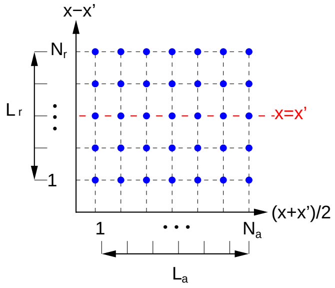

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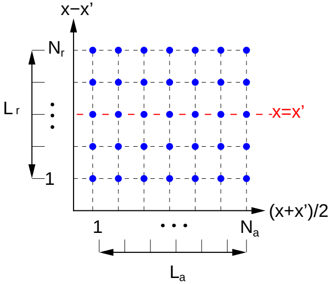

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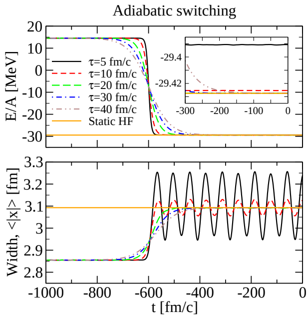
Traditional vs. rotated evolutions

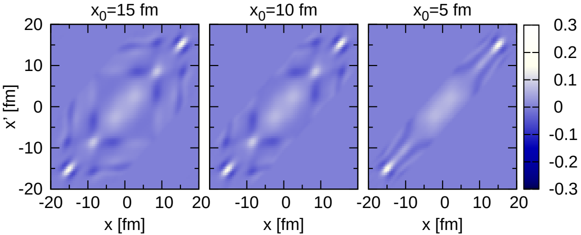
Research program



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

- Used adiabatic theorem to solve mean-field √
- Full (N_x^2), damped & cut $(N_a \times N_r)$ 1D mean-field evolution √
- Identified lack of correlations in Wigner distribution √
- Full 1D correlated evolution: Born approximation ∼ √

Research program



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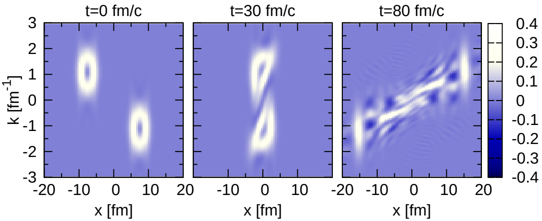
Research program

Wigner distribution



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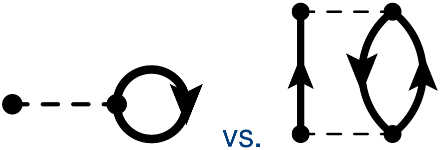
Research program



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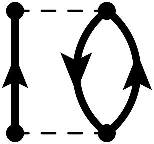
Time evolution beyond the mean-field

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



- Direct Born approximation $\Rightarrow$ simplest conserving approximation
- FFT to compute convolution integrals
- Collision integrals $\Rightarrow$ memory effects in 2D $\Rightarrow (t, t')$
- First benchmark calculation to get acquainted with methodology

Time evolution beyond the mean-field

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

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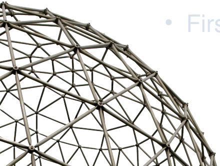

Time evolution beyond the mean-field

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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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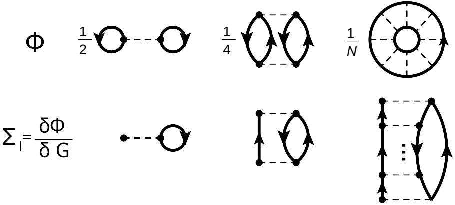
Time evolution beyond the mean-field



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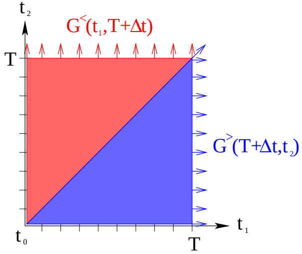
Two time Kadanoff-Baym equations

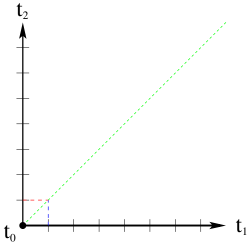
- Time off-diagonal time elements are present
- Need of a strategy to deal with memory & two-times
- Use symmetries $\mathcal{G}^{\lessgtr}(\mathbf{1},\mathbf{2}) = -[\mathcal{G}^{\lessgtr}(\mathbf{2},\mathbf{1})]^*$ to minimize resources
- Self-consistency imposed at every time step



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



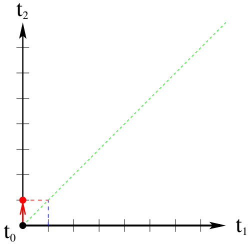
$$\mathcal{G}^<(t_1, T+\Delta t) = e^{i\varepsilon\Delta t}\mathcal{G}^<(t_1, T) - \varepsilon^{-1}\left(1 - e^{i\varepsilon\Delta t}\right)\overline{I_2^<(t_1, T+\Delta t)}$$

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

$$\mathcal{G}^<(T+\Delta t, T+\Delta t) = e^{i\varepsilon\Delta t}\left[\mathcal{G}^>(T,T) - \overline{I_1^<(T+\Delta t)} - \overline{I_2^<(T+\Delta t)}\right]e^{-i\varepsilon\Delta t}$$

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

Strategy to solve two-time equations



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

$$\mathcal{G}^{<}(T+\Delta t, T+\Delta t) = e^{i\varepsilon\Delta t}\left[\mathcal{G}^{>}(T, T) - \overline{I_1^{<}(T+\Delta t)} - \overline{I_2^{<}(T+\Delta t)}\right]e^{-i\varepsilon\Delta t}$$

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Strategy to solve two-time equations

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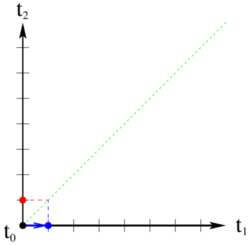

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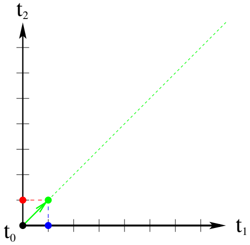
Strategy to solve two-time equations



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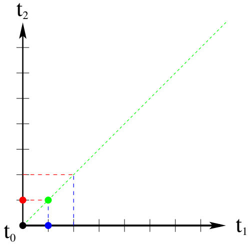

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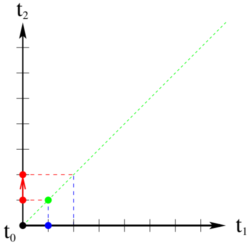

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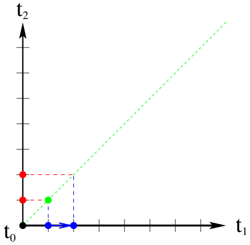

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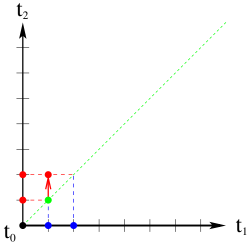

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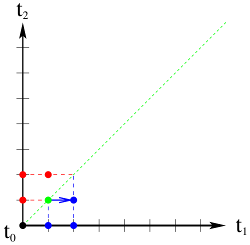

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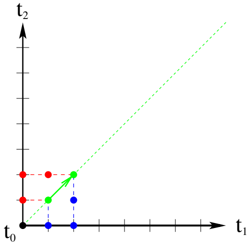

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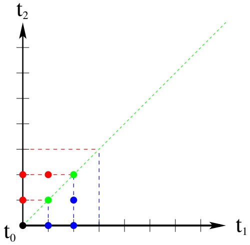

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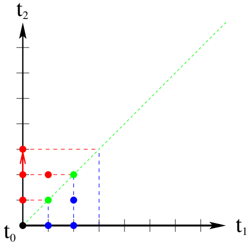

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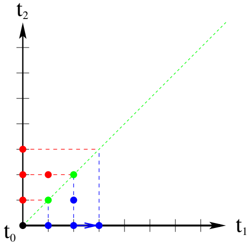

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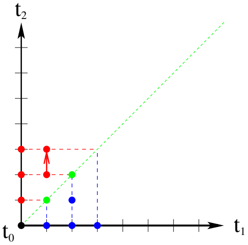

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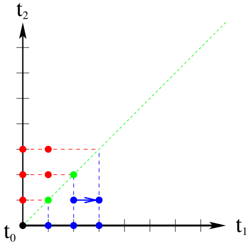

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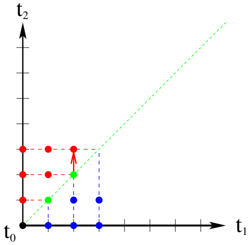

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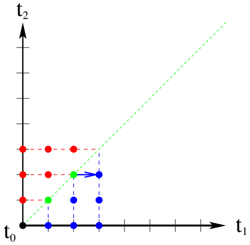

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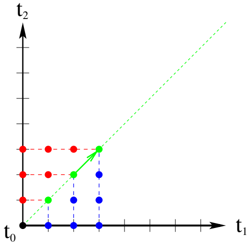

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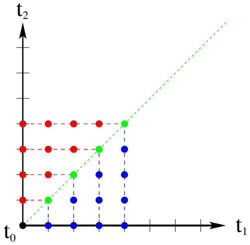

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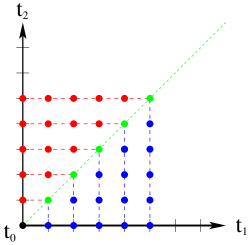

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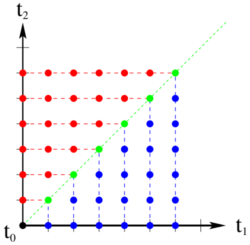

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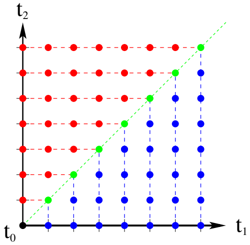

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Nuclear time-dependent correlations

- Some experience already gathered for uniform systems

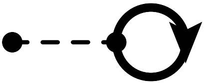
  Danielewicz, Ann. Phys. 152, 239 (1984)

  H. S. Köhler, PRC 51 3232 (1995)

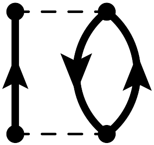
- Expected physical effects
  - Thermalization $(0 < n_\alpha < 1)$
  - Damping of collective modes
- Correlations in the initial state
  - Will a mean-field system evolve to a correlated ground state?
  - Adiabatic switching on of correlations?
  - Imaginary time evolution to get ground states?
- Testing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



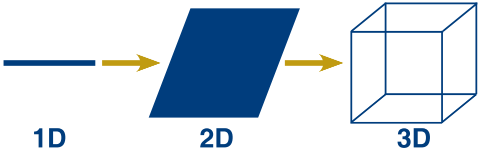
vs.



- Used adiabatic theorem to solve mean-field $\surd$
- 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

UNIVERSITY OF SURREY



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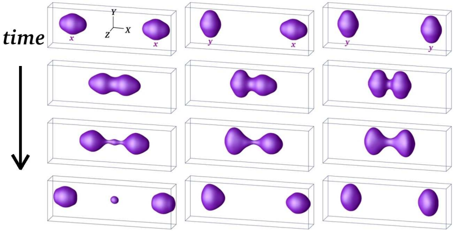

Golabek & Simenel, Phys. Rev. Lett. **103**, 042701 (2009)

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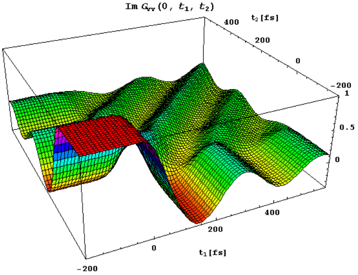
Nuclear Kadanoff-Baym

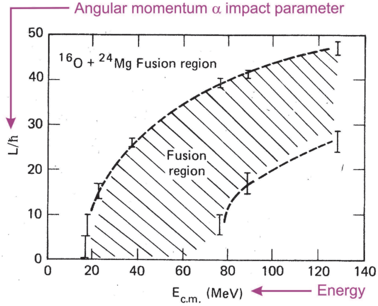
Potential & challenges



- Potential for applications in nuclear reactions & structure
- Microscopic understanding of dissipation
- Response for nuclei including collision width
- Multidisciplinary research: from quantum dots to cosmology!

Nuclear Kadanoff-Baym

Potential & challenges



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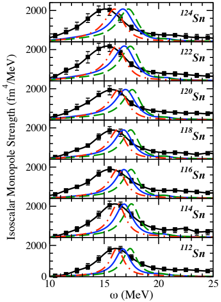

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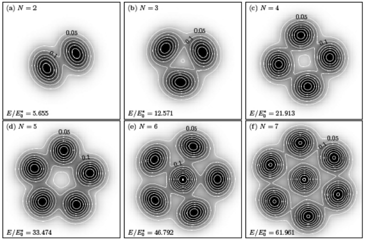

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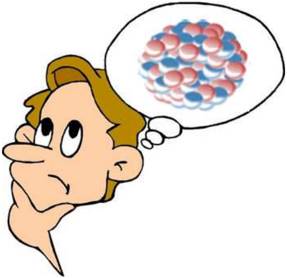
Thank you!



MARIE CURIE ACTIONS

PEOPLE

Science & Technology Facilities Council