Quantum transport in many-body systems

Towards a Kadanoff-Baym approach for nuclear reactions

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M. Buchler

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Outline

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1 Green's functions in & out of equilibrium

2 Statics: mean-field theory

3 Statics: beyond mean-field

4 Dynamics: mean-field

5 Dynamics: Kadanoff-Baym results

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Statics

SCGF

- In equilibrium
  - Thermal properties
  - Transport coefficients
- Finite temperature
  - Phase transition
  - Critical exponents
- Beyond mean-field
  - Momentum distribution
  - Knock-out reactions
- Collisions vs correlations

Many-body Green's functions

Dynamics

Kadanoff-Baym

- Out of equilibrium
  - Thermalization times
  - Quantum transport
- Thermalization
  - Phase transition
  - Universality classes
- Fluctuations
  - Yields
  - Stopping
- Collisions

Equilibrium Green's functions

A powerful tool

$$i^N \mathcal{G}(\mathbf{1},\ldots,\mathbf{N};\mathbf{1}',\ldots,\mathbf{N}') = \left\langle \mathcal{T}\left\{ a(\mathbf{1})\cdots a(\mathbf{N}) a^\dagger(\mathbf{N}')\cdots a^\dagger(\mathbf{1}') \right\} \right\rangle$$

$\langle\cdot\rangle \to$ average over states

$\mathcal{T} \to$ some sort of time ordering (real, imaginary, on the contour...)

$\mathbf{1} \to \mathbf{r}_1, t_1, \sigma_1, \tau_1$

- Definition of N-body Green's functions
- Gives access to all N-body operators
- Primary advantage: diagrammatic representation
- Complex processes in dense media $\Rightarrow$ Correlations

Dickhoff & van Neck, *Many-body theory exposed!*

Equilibrium Green's functions

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

$$\mathcal{G}^{<}(x, x'; t - t') = i \left\langle a^{\dagger}(x', t') a(x, \tau) \right\rangle$$

$$\mathcal{G}^{>}(x, x'; t - t') = -i \left\langle a(x, \tau) a^{\dagger}(x', t') \right\rangle$$

$$\mathcal{G}^{T}(x, x'; t - t') = -i \left\langle T[a(x, \tau) a^{\dagger}(x', t')] \right\rangle$$

$$\mathcal{G}^{R}(x, x'; t - t') = \Theta(\tau) \left[\mathcal{G}^{>}(x, x'; t - t') - \mathcal{G}^{<}(x, x'; t - t') \right]$$

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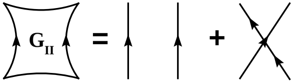

$$\mathcal{G}_{II}(\mathbf{1},\mathbf{2};\mathbf{1}',\mathbf{2}') = \mathcal{G}(\mathbf{1},\mathbf{1}')\mathcal{G}(\mathbf{2},\mathbf{2}') - \mathcal{G}(\mathbf{1},\mathbf{2}')\mathcal{G}(\mathbf{1}',\mathbf{2})$$

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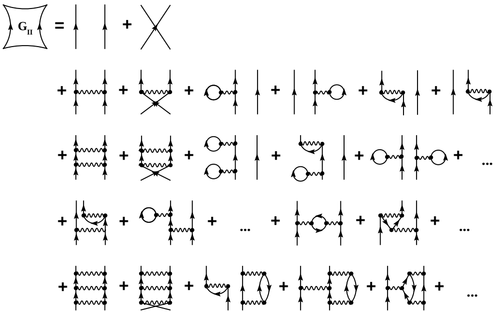

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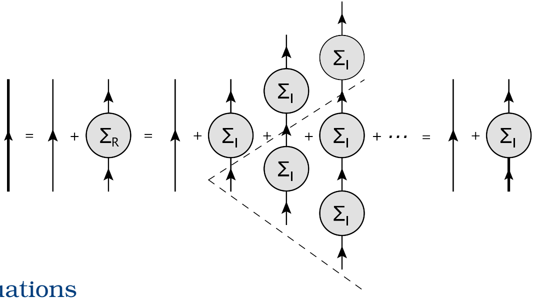
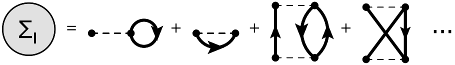


Dyson Equations

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

$$\left\{ -i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} \right\} \mathcal{G}(\mathbf{1},\mathbf{1}') = \delta(\mathbf{1},\mathbf{1}') + \int \mathrm{d}\mathbf{2}\, \mathcal{G}(\mathbf{1},\mathbf{2})\Sigma(\mathbf{2},\mathbf{1}')$$

Equilibrium Green´s functions



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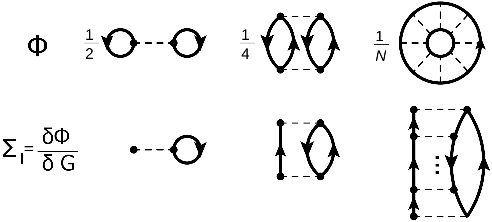

Baym, Phys. Rev. 127, 1391 (1962)

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Consistent choice of diagrams

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

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

Kadanoff-Baym equations

Non-equilibrium Green's functions

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

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

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- Evolution of non-equilibrium systems from general principles
- Include dissipation and memory effects, via self-energies
- Complicated numerical solution, but very universal framework
- Simulations preserve symmetries and conserve energy

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

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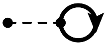
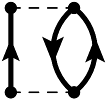
Mean-field

$\Sigma_{HF} \Rightarrow$ 

Beyond mean-field

$\Sigma^{\lessgtr} \Rightarrow$ 

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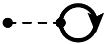
$\Sigma_{HF} \Rightarrow$ 

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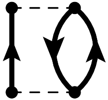
$\Sigma^{\lessgtr} \Rightarrow$ 

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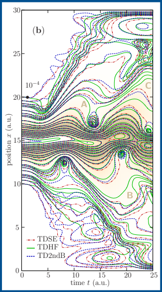
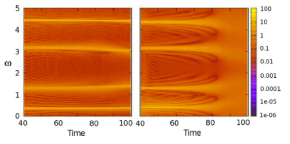
Non-equilibrium Green's functions

Atoms & molecules



Dahlen, van Leeuwen, PRL **98**, 153004 (2007)
Balzer, Bonitz et al., PRA **81**, 022510 (2010)
Balzer, Bonitz et al., PRA **82**, 033427 (2010)

Transport in nanostructures



Stefanucci & Almbladh, JPG **35**, 17 (2006)
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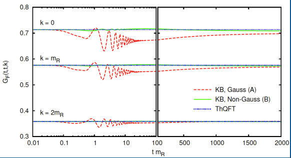
Nonequilibrium QFT



Aarts & Berges, PRD 64, 105010 (2001)
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Berges et al., PRL **100**, 085011 (2009)
Kronenwett & Gasenzer, APB **102**, 469 (2011)

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KB & classical Langevin processes

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Classical Langevin equation with finite memory

$$M\ddot{x} + 2\int_{-\infty}^{t} d\bar{t}\,\Gamma(t-\bar{t})\dot{x}(\bar{t}) = \xi(t)$$

- Friction kernel, $\Gamma(t)$ is well behaved: $\Gamma(\omega) \geq 0$ & finite
- Time correlation given by colored noise

$$I(t-t') = \langle\langle \xi(t)\xi(t') \rangle\rangle = 2T\Gamma(t-t')$$

- Define retarded Green's functions

$$\dot{G}_{ret}(t) = \delta(t) + \frac{2}{m}\int_{-\infty}^{t} d\bar{t}\,\Gamma(t-\bar{t})G_{ret}(t')$$

- FDT is fulfilled!

$$\langle\langle p^2 \rangle\rangle \xrightarrow[t\to\infty]{} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\, G_{ret}(\omega)I(\omega)G_{adv}(\omega) = TM$$

Greiner & Leupold, Ann. Phys. **270**, 328 (1998)

KB & quantum Langevin processes

quantum Langevin equation with finite memory

$$M\ddot{\phi} + 2\int_{-\infty}^{t} d\bar{t}\,\Gamma(t-\bar{t})\dot{\phi}(\bar{t}) = \xi(t)$$

- High-energy modes as thermal bath of low energy
- $\Gamma \sim Im\Sigma$ couples ϕ to bath of HE modes
- Stochastic quations arise from KB
- Fluctuations are quantal!

$$\frac{\Delta N}{N} \sim \frac{3}{2} T\varepsilon_F$$

- or:

$$\Delta N \neq n_F(1-n_F)$$

- Quantum & finite T fluctuations used in reactions!

$$\frac{\sigma_{xy}^2}{N} = \frac{16m^2\varepsilon_F^2}{35}\left[1+\frac{7\pi^2}{6}\left(\frac{T}{\varepsilon_F}\right)^2\right]$$

Greiner & Leupold, Ann. Phys. **270**, 328 (1998)

Zheng & Bonasera, Phys. Lett. B **696**, 178 (2011)

Outline

Mean-field level calculations

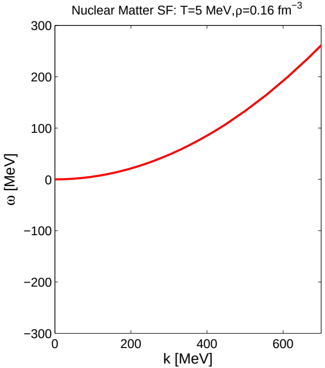
Fixed T & ρ - Micro properties

$$\varepsilon_k = \frac{k^2}{2m}$$

$$n_k = \frac{1}{1 + e^{\beta(\varepsilon_k - \mu)}}$$

$$\updownarrow$$

$$\rho = \sum_k n_k(\mu)$$



Bulk properties

$$e = \sum_k \frac{k^2}{2m} n_k + \frac{1}{2} \sum_k U(k) n_k$$

$$s = -\sum_k n_k \ln n_k + (1 - n_k) \ln[1 - n_k]$$

- Free fermions
- Mean-field approximation: sp spectrum

Mean-field level calculations

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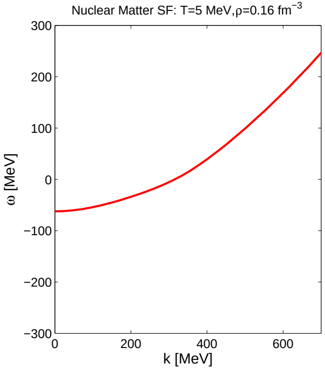

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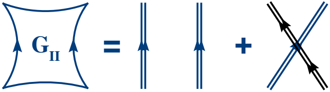
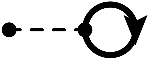


$\Sigma =$ 

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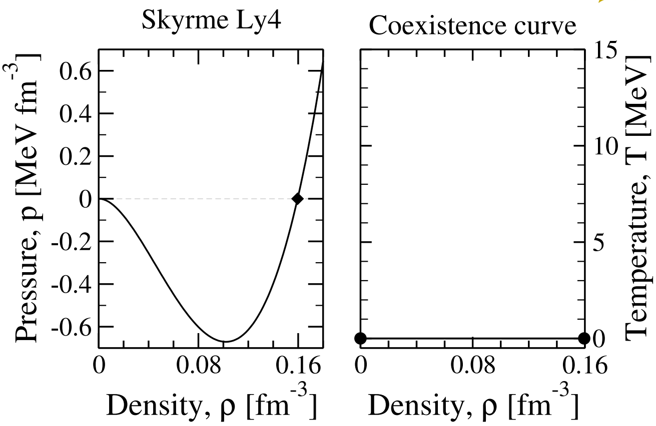
Self-consistent mean-field solution

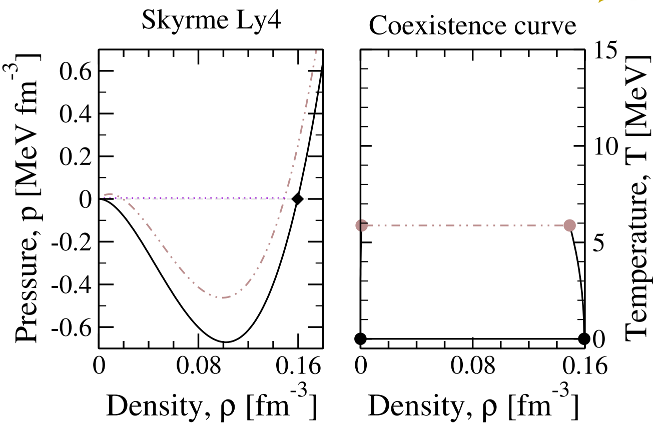


Maxwell's criterion $p_g = p_l \qquad \mu_g = \mu_l$

- Describes simultaneously liquid & gas
- Three points stand out

A. Rios, Nucl. Phys. A **845**, 58 (2010)

Self-consistent mean-field solution



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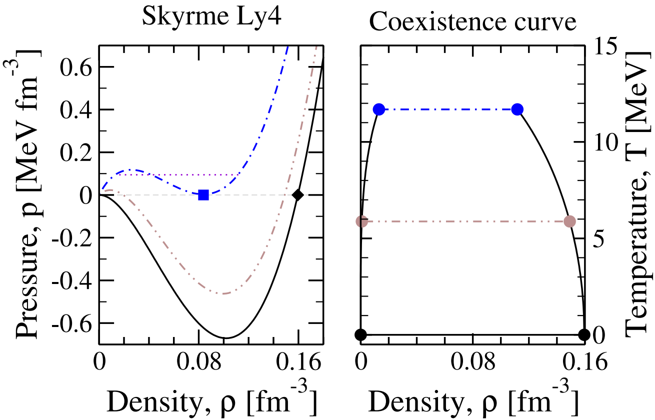

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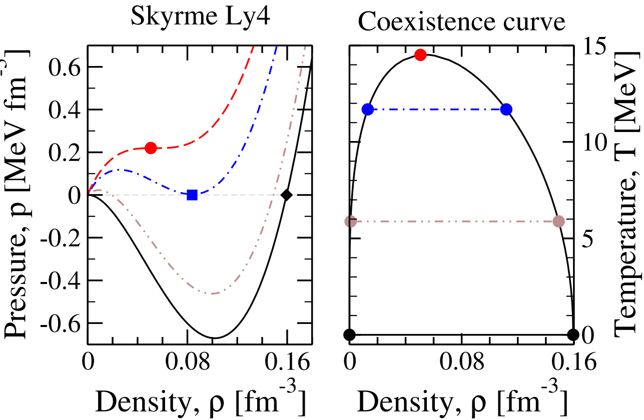

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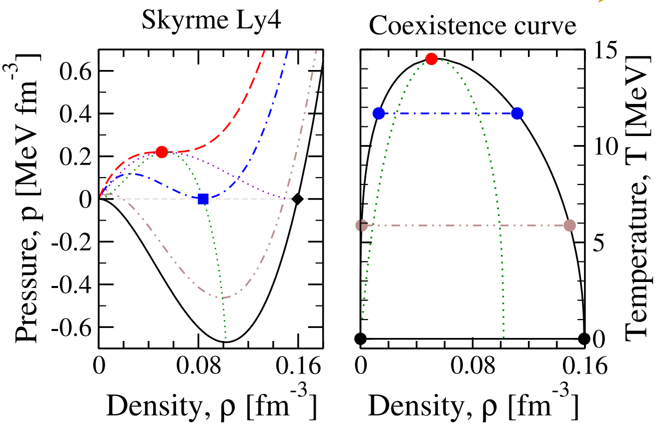

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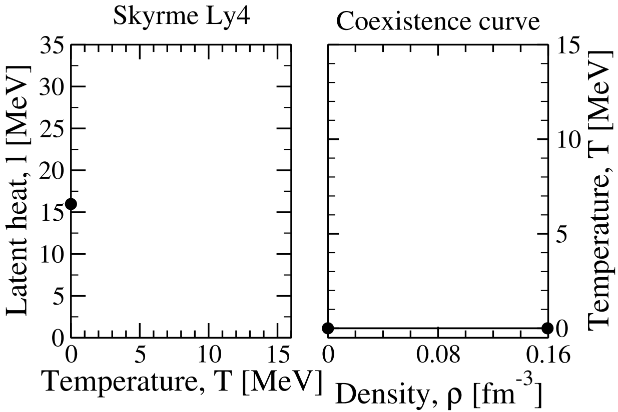
Latent heat



$$l = T(s_g - s_l)$$

$$l = T\left(\frac{1}{\rho_g} - \frac{1}{\rho_l}\right) \left.\frac{\mathrm{d}p}{\mathrm{d}T}\right|_{\mathrm{coex}}$$

- Low temperature limit: $l \sim e_0 + \frac{5}{2}T$
- Intermediate maximum!? $l \sim 30$ MeV
- Critical behavior: $l \sim (T_c - T)^{1/2}$

A. Carbone, A. Polls, A. Rios, I. Vidaña, Phys. Rev. C **83**, 024308 (2011)

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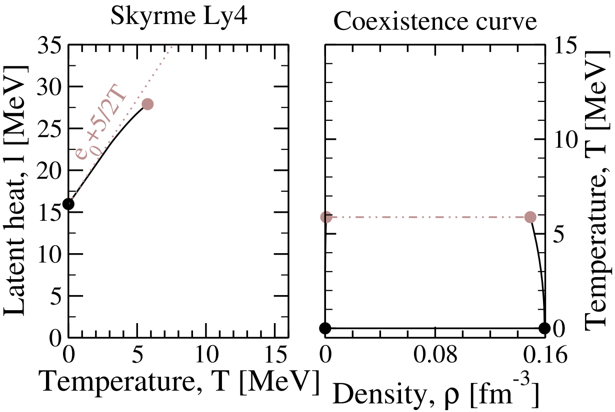

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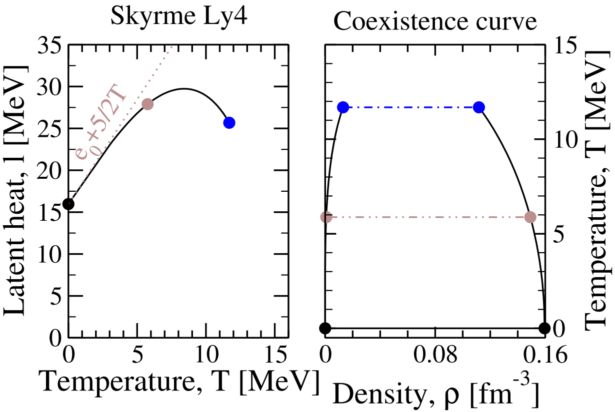

$$l = T(s_g - s_l)$$

$$l = T\left(\frac{1}{\rho_g} - \frac{1}{\rho_l}\right) \left.\frac{\mathrm{d}p}{\mathrm{d}T}\right|_{\mathrm{coex}}$$

- Low temperature limit: $l \sim e_0 + \frac{5}{2}T$
- Intermediate maximum!? $l \sim 30$ MeV
- Critical behavior: $l \sim (T_c - T)^{1/2}$

A. Carbone, A. Polls, A. Rios, I. Vidaña, Phys. Rev. C **83**, 024308 (2011)

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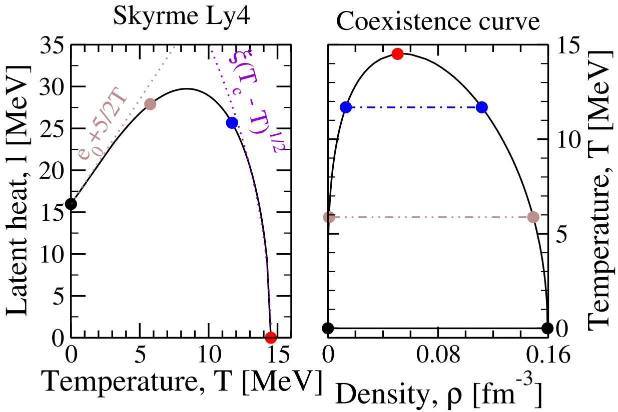

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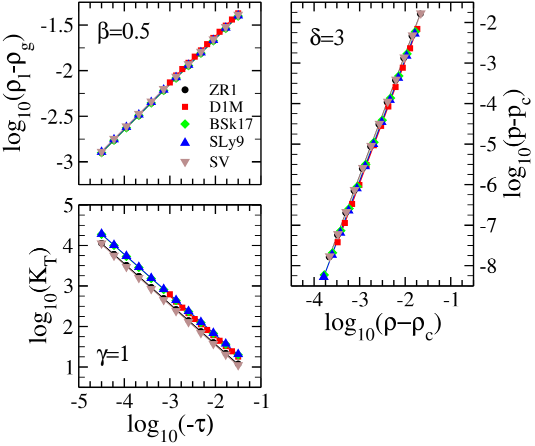
A. Carbone, A. Polls, A. Rios, I. Vidaña, Phys. Rev. C **83**, 024308 (2011)

Critical exponents

Determination of critical exponents



A. Rios, Nucl. Phys. A **845**, 58 (2010)

$$\rho_l - \rho_g \sim (-\tau)^{\beta}$$

$$K_T = \rho \left.\frac{\partial p}{\partial \rho}\right|_T \sim (-\tau)^{\gamma}$$

$$|p(\rho, T_c) - p_c| \sim |\rho - \rho_c|^{\delta}$$

Hartree-Fock

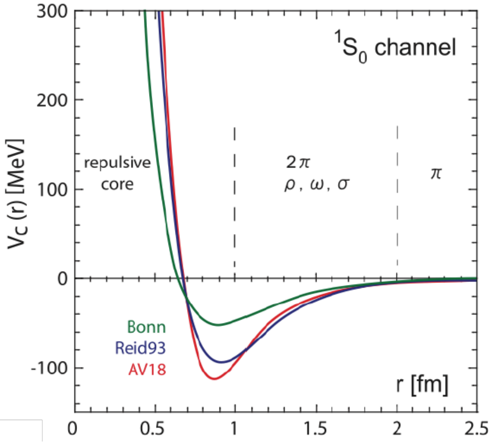
$$\langle \rho(1,2) \rangle \sim \langle \rho(1) \rangle \langle \rho(2) \rangle$$

Lack of micro fluctuations!

Collisions/correlations?

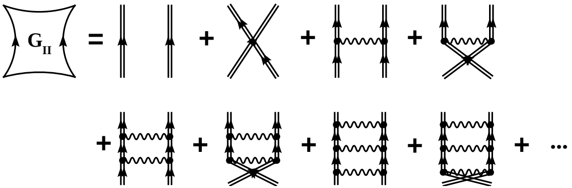
Outline

Ladder SCGF



- Ab initio approach from microscopic NN interactions
- Impose self-consistency & full off-shell effects
- Finite temperature: avoid pairing instability
- Consistency: between micro- and macroscopic properties

Ladder SCGF



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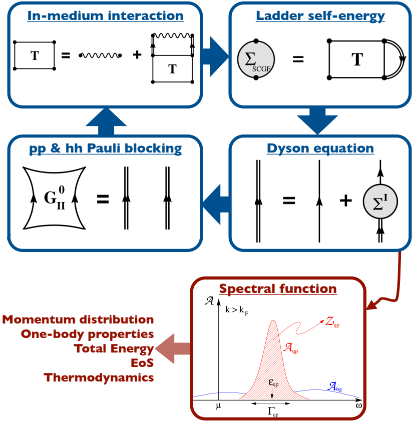
Ladder SCGF

Ladder approximation within SCGF



Ramos, Polls & Dickhoff, NPA **503** 1 (1989)
Alm *et al.*, PRC **53** 2181 (1996)
Dewulf *et al.*, PRL **90** 152501 (2003)
Frick & Müther, PRC **68** 034310 (2003)
Rios, PhD Thesis, U. Barcelona (2007)
Somà & Bożek, PRC **78** 054003 (2008)

- Ab initio approach from microscopic NN interactions
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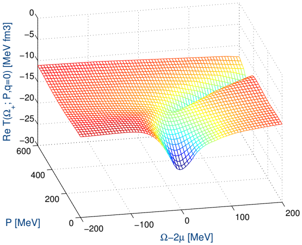
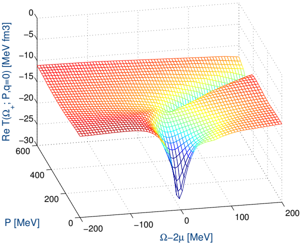
Ladder SCGF

In-medium T-matrix
T=20 MeV



In-medium T-matrix
T=5 MeV



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Ladder SCGF

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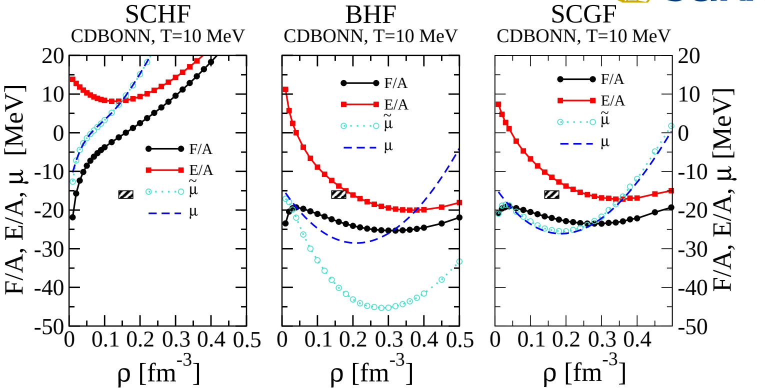

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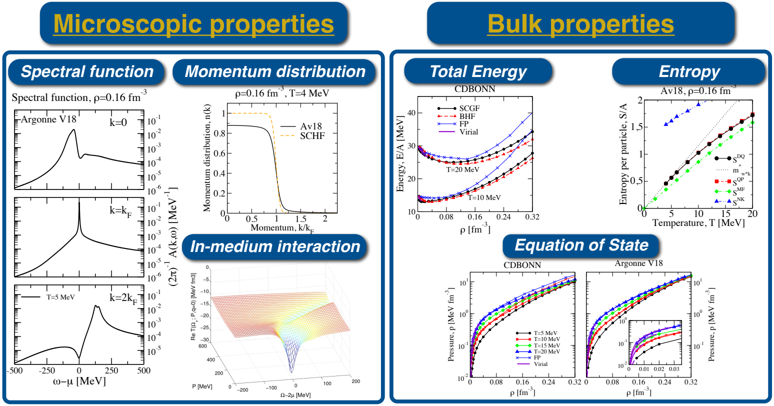
Ladder SCGF

Ladder approximation



- Ab initio approach from microscopic NN interactions
- Impose self-consistency & full off-shell effects
- Finite temperature: avoid pairing instability
- Consistency: between micro- and macroscopic properties

Correlations & spectral function

Fixed T & ρ

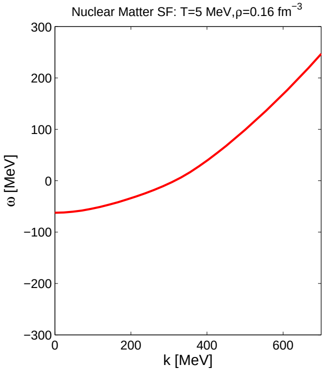
$$\varepsilon_k = \frac{k^2}{2m} + U(k)$$

$$n_k = \frac{1}{1+e^{\beta(\varepsilon_k-\mu)}}$$

$$\updownarrow$$

$$\rho = \sum_k n_k(\mu)$$

$$s = -\sum_k n_k \ln n_k + (1-n_k)\ln[1-n_k]$$



- Mean-field fermions
- Spectral function & sp strength
- SRC strength measured in light nuclei

Correlations & spectral function

Spectral function

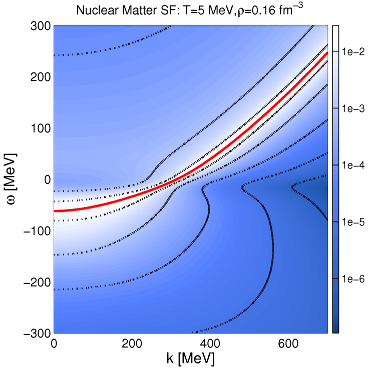
$$\mathcal{A}^{<}(k,\omega) = \sum_{n,m} \frac{e^{-\beta(E_n-\mu A)}}{Z} \left|\langle m|a_{\mathbf{k}}|n\rangle\right|^2 \delta\left[\omega - (E_n^A - E_m^{A-1})\right]$$

Momentum distribution

$$n_k = \int \frac{\mathrm{d}\omega}{2\pi} f(\omega)\mathcal{A}(k,\omega)$$

Probability

$$\int \frac{\mathrm{d}\omega}{2\pi}\, \mathcal{A}(k,\omega) = 1$$



- Mean-field fermions
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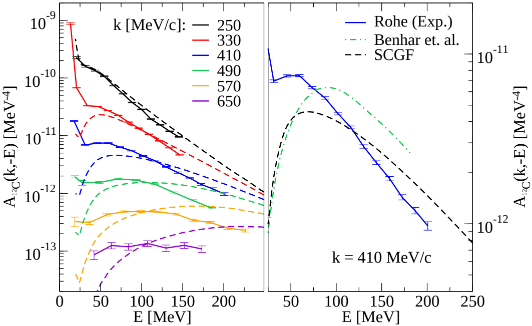
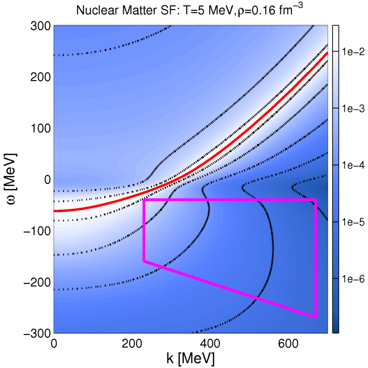
Correlations & spectral function

^{12}C spectral function from $(e, e'p)$



Rohe *et al.*, PRL **93** 182501 (2004)



- Mean-field fermions
- Spectral function & sp strength
- SRC strength measured in light nuclei

Momentum distribution

Correlated one-body observable

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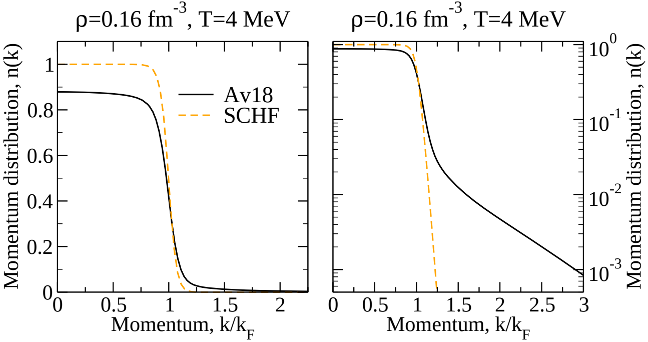
$$n(k) = \langle \hat{a}^\dagger_k \hat{a}_k \rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \mathcal{A}(k,\omega) f(\omega)$$



- 15% depletion at low k, population at high k
- Thermalization & correlations have similar impact

Momentum distribution

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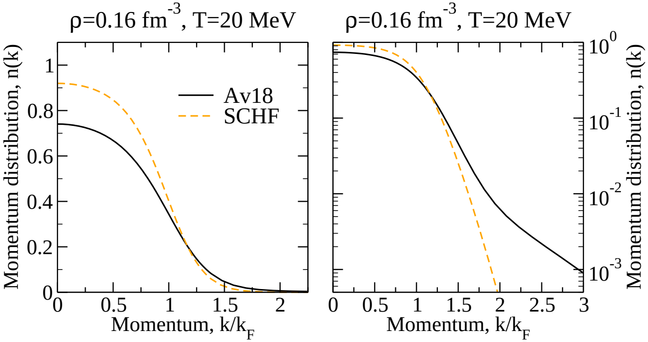

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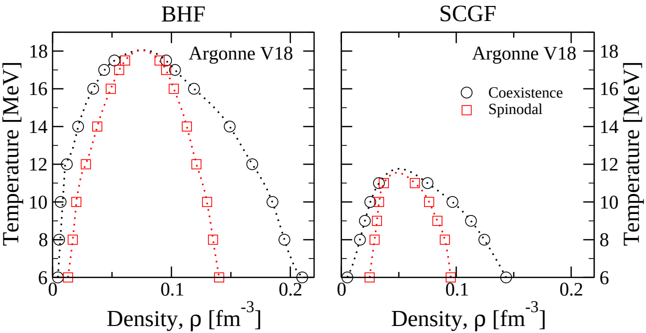
Liquid-gas phase transition



Potential	Approach	T_f (MeV)	T_c (MeV)	ρ_c (fm^{-3})	p_c (MeV fm^{-3})	$\frac{p_c}{T_c \rho_c}$
Argonne V18	SCGF	9.5	11.6	0.05	0.08	0.14
	BHF	13.1	18.1	0.08	0.40	0.28
CDBONN	SCGF	14.4	18.5	0.11	0.40	0.20
	BHF	17.2	23.3	0.11	0.73	0.28

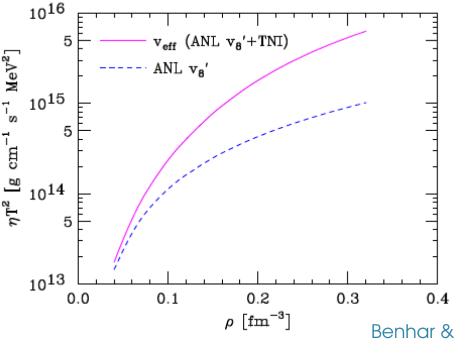
- $T_c^{BHF} > T_c^{SCGF} \Rightarrow$ different critical behaviour!
- No clusterization or three-body forces! $\Rightarrow$ upper estimate

A. Rios *et al.*, PRC **78**, 044314 (2008)

Towards ab initio transport (static!)

- Don't stick to EoS only, aim at complete NS models!
- Better if experimentally testable
  1. Mean-free path
  2. Viscosities
  3. Neutrino responses
  4. Specific heat

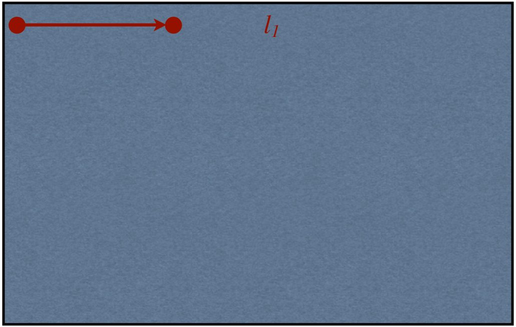
Shear viscosity of neutron matter



Benhar & Valli, PRL **99**, 232501 (2007)

Classical mean-free path

Moving particles in a medium



- Average distance travelled in medium
- Medium density dependence
- Particle energy dependence

$$\lambda_k = \frac{1}{\rho} \frac{1}{\sigma_k}$$

Classical mean-free path

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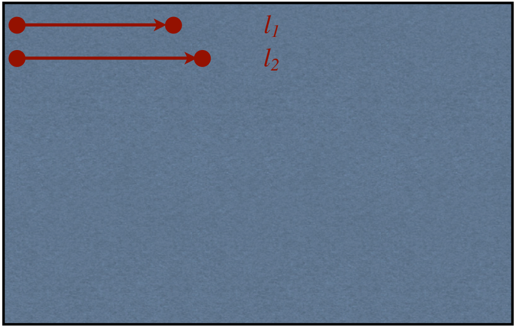
Moving particles in a medium



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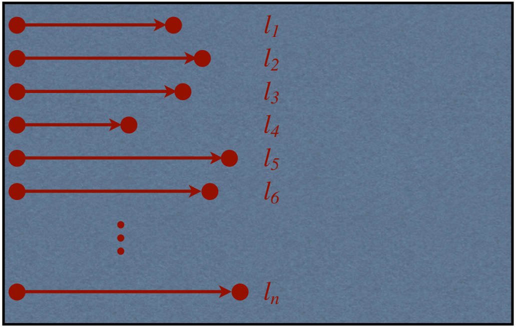


$$\lambda = \frac{l_1 + l_2 + \cdots + l_n}{n}$$

- Average distance travelled in medium
- Medium density dependence
- Particle energy dependence

$$\lambda_k = \frac{1}{\rho}\frac{1}{\sigma_k}$$

Quantum mean-free path

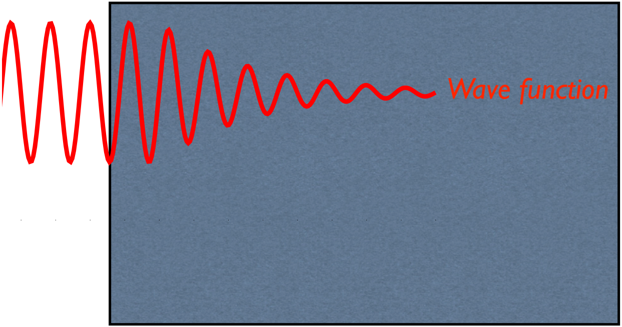
Moving wave packets in a medium

- Average distance travelled in medium
- Medium density dependence
- Particle energy dependence

$$\lambda_k = ?$$

Quantum mean-free path

Moving wave packets in a medium



- Average distance travelled in medium
- Medium density dependence
- Particle energy dependence

$\lambda_k = ?$

Quantum mean-free path

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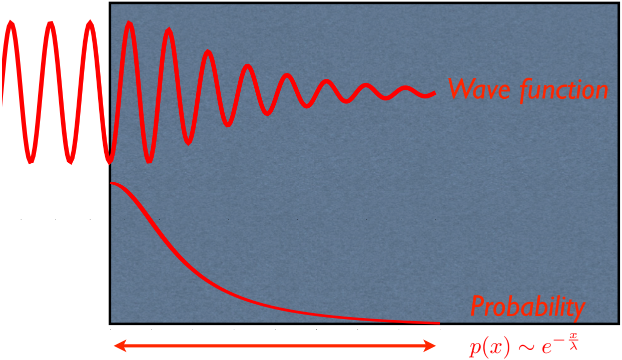
Moving wave packets in a medium



- Average distance travelled in medium
- Medium density dependence
- Particle energy dependence

$\lambda_k = ?$

Damping in the medium

"Naive" optical potential model

$$\left[-\frac{\nabla^2}{2m} + \mathrm{Re}\,\Sigma(\varepsilon_k) + i\mathrm{Im}\,\Sigma(\varepsilon_k)\right]\psi(\mathbf{r}) = \varepsilon_k \psi(\mathbf{r})$$

$$\psi(r) = N e^{-i\left\{k + \frac{i}{2\lambda_k}\right\} r}$$

$$\lambda_k = -\frac{k}{2m}\frac{1}{\mathrm{Im}\,\Sigma(\varepsilon_k)} = \frac{k}{m}\frac{1}{\Gamma_k}$$

$$k^2 \sim 2m\left[\varepsilon_k + \mathrm{Re}\,\Sigma(\varepsilon_k)\right]$$

- Ambiguity in definition of Γ_k and ε_k due to many-body
- Space non-locality $\Rightarrow$ self-energy depends on k, $\Sigma(k,\omega)$
- Time non-locality $\Rightarrow$ self-energy depends on ω, $\Sigma(k,\omega)$

Previous calculations

$$\lambda_k = \frac{v_k}{\Gamma_k} = \frac{1}{\Gamma_k}\frac{\partial \varepsilon_k}{\partial k}$$

- Exact solution only possible in complex plane

$$z_k = \frac{k^2}{2m} + \mathrm{Re}\,\Sigma(k, z_k) + i\mathrm{Im}\,\Sigma(k, z_k)$$
$$\varepsilon_k = \mathrm{Re}\, z_k \qquad \Gamma_k = \mathrm{Im}\, z_k$$

- Need to know complex self-energy (impossible?)
- Expand on imaginary part of argument:

$$\mathrm{Re}\,\Sigma(\varepsilon_k + i\Gamma_k) \sim \mathrm{Re}\,\Sigma(\varepsilon_k) + i\Gamma_k \left.\frac{\partial \mathrm{Re}\,\Sigma'(\omega)}{\partial \omega}\right|_{\omega=\varepsilon_k} + \mathcal{O}(\Gamma_k^2)$$
$$\mathrm{Im}\,\Sigma(\varepsilon_k + i\Gamma_k) \sim \mathrm{Im}\,\Sigma(\varepsilon_k) + i\Gamma_k \left.\frac{\partial \mathrm{Im}\,\Sigma'(\omega)}{\partial \omega}\right|_{\omega=\varepsilon_k} + \mathcal{O}(\Gamma_k^2)$$

& solve quasi-particle equation at different orders

Calculation of the mean free path

- Approximation schemes proposed previously
  - First renormalization

$$\varepsilon_1(k) = \frac{k^2}{2m} + \mathrm{Re}\tilde{\Sigma}(k, \varepsilon_1(k)) \qquad \Gamma_1(k) = \mathrm{Im}\,\tilde{\Sigma}(k, \varepsilon_1(k))$$

  - Second renormalization

$$\varepsilon_2(k) = \varepsilon_1(k) - \mathrm{Im}\,\tilde{\Sigma}(k, \varepsilon_1(k))\,\mathrm{Im}\,\frac{1}{1 - \tilde{\Sigma}'(z_1(k))}$$

$$\Gamma_2(k) = \Gamma_1(k)\,\mathrm{Re}\,\frac{1}{1 - \tilde{\Sigma}'(z_1(k))}$$

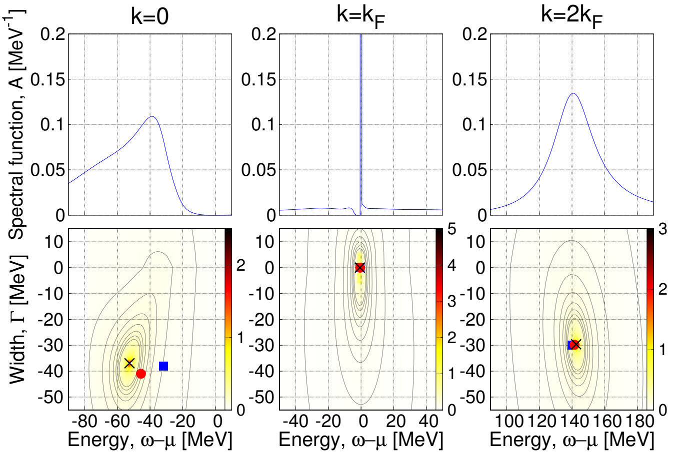
  - Nuclear renormalization

$$\varepsilon_{2'}(k) = \varepsilon_1(k) \qquad \Gamma_{2'}(k) = \Gamma_1(k)\frac{1}{1 - \mathrm{Re}\tilde{\Sigma}'(\varepsilon_1(k))}$$

    - Negele *et al.* in the 80's reconcile experiments
  - We want to get rid of the expansion!

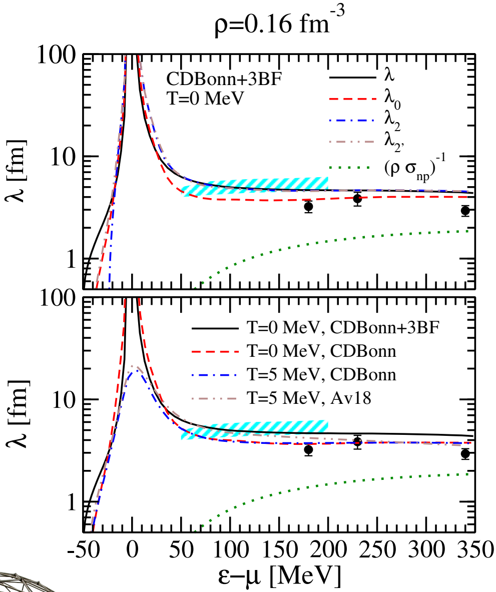
Hunting the pole

CDBonn, $T = 0$, $\rho = 0.16\ \mathrm{fm}^{-3}$



- Cross: correct pole
- Square: first renormalization
- Circle: second renormalization
- Infinite λ at k_F due to Luttinger's theorem

Nucleon mean-free path



$$\lambda_k = \frac{k}{m_k^* \Gamma_k}$$

- At zero T, infinite λ at Fermi surface
- $\lambda \sim 4 - 5$ fm above 50 MeV
- Compatible with experimental pA data
- Classical approximation is invalid!

- Little effect of temperature
- Little effect of 3BFs
- At finite T, finite λ at Fermi surface

A. Rios & V. Somà, Phys. Rev. Lett. **108**, 012501 (2012)

Outline

First principles in nuclear dynamics

	Nuclear structure	Nuclear reactions
 Phenomenological	• Fit effective interactions to stable nuclei • Rely on Hartree-Fock approximation • Extrapolate exotic nuclei • Fastest way to objective	Time Dependent Hartree-Fock
 First principles	• Microscopic NN force • Use many-body theory to describe nuclear medium • Build exotic nuclei • Safest way to objective	?

Limitations of the mean-field

Frictionless

Dissipative

Effect	Observable	Mean-field	Kadanoff-Baym
Many-body trajectory	Sub-barrier fusion	✔	✔
One-body dissipation	Transfer probability	✔	✔
Two-body dissipation	Stopping	✘	✔
Fluctuations	Yields	✘	✔
Collisions	Resonance widths	✘	✔

Research program

New first principles frameworks

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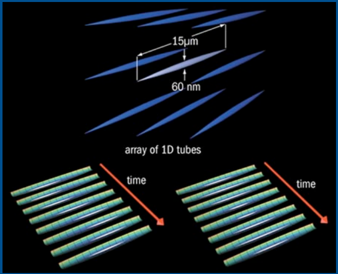
Kadanoff-Baym

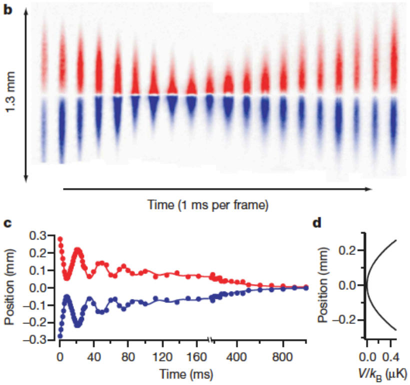
- *Full 1D simulations*
- *Test numerical propagation schemes*
- *Assessment of many-body approximations*

1D ultracold gases



- Start with 1D systems
- Many-body dynamics of ultracold atoms
- Progressive understanding of higher D

Collisions of spin ↑ & ↓ ^{6}Li atom clouds



Sommer *et al.*, Nature 472, 201 (2011)

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New first principles frameworks

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Kadanoff-Baymt

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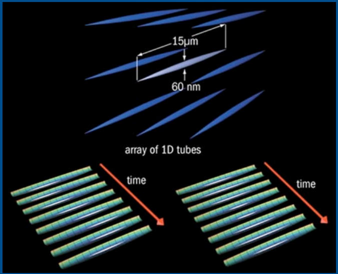
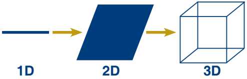
1D ultracold gases



Nuclear physics



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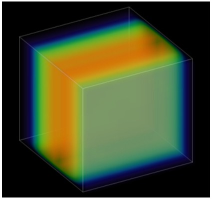
Collisions of 1D slabs



- Frozen y, z coordinates, dynamics in x
- Simple zero-range mean field:

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

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

Collisions of 1D slabs: fusion

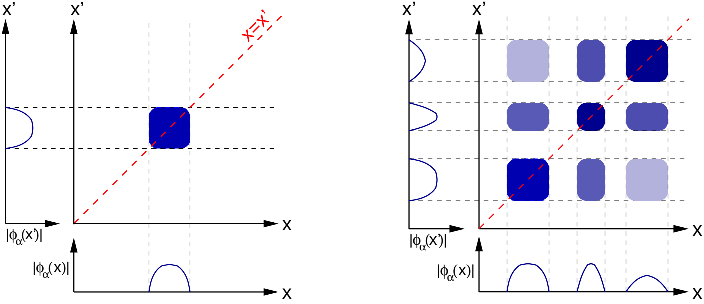
$$-i\mathcal{G}^<(x,x') = \sum_{\alpha<F} \phi_\alpha(x)\phi_\alpha(x') \quad \Rightarrow \quad \mathcal{G}^<(x,x',P) = e^{iPx}\mathcal{G}^<(x,x',P=0)e^{-iPx'}$$

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

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

Off-diagonal elements: origin

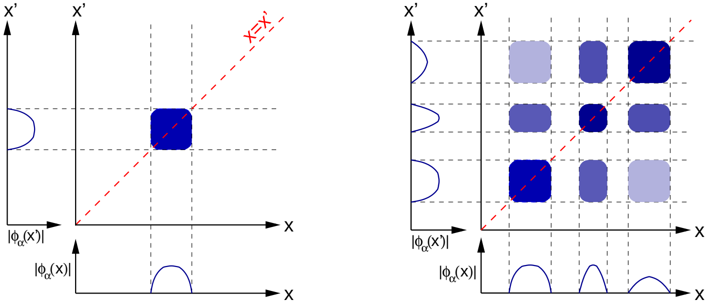
$$-i\mathcal{G}^{<}(x,x') = \sum_{\alpha<F} \phi_\alpha(x)\phi^*_\alpha(x')$$



Correlation between single-particle states that are far away!

Off-diagonal elements: origin

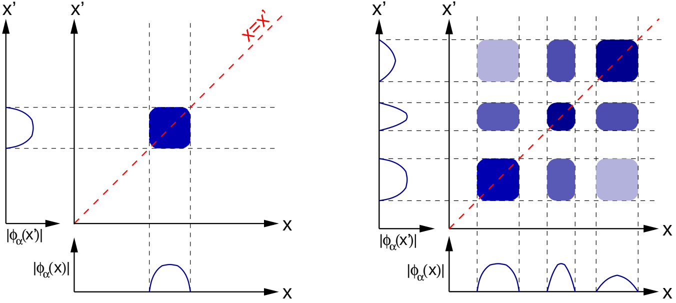
$$-i\mathcal{G}^{<}(x,x') = \sum_{\alpha<F} \phi_\alpha(x)\phi^*_\alpha(x')$$



Correlation between single-particle states that are far away!

Multifragmentation

Off-diagonal elements: origin



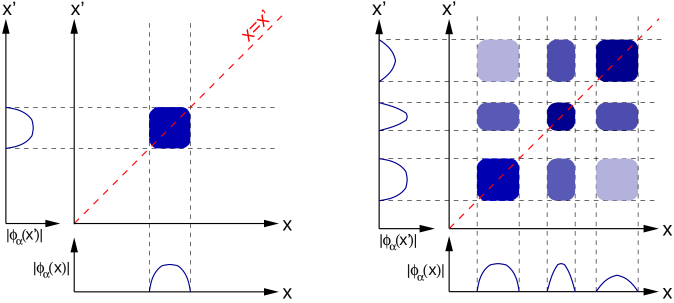
- Off-diagonal elements describe correlation of single-particle states

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

- Diagonal elements yield physical properties

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

Off-diagonal elements: importance



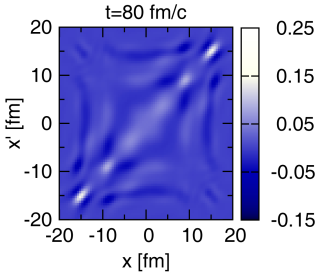
Conceptual issues:

- 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: filtering out



- Can we filter off-diagonal elements without perturbing diagonal evolution?
- Super-operator filter: act in two positions of $\mathcal{G}^<$ instantaneously
- Use an imaginary super-operator 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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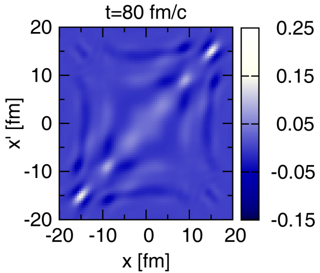

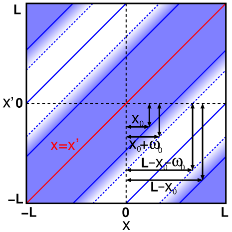

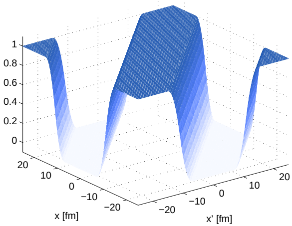

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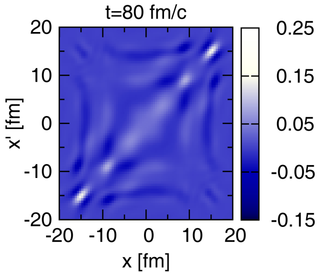

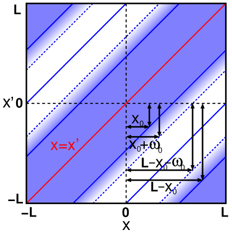

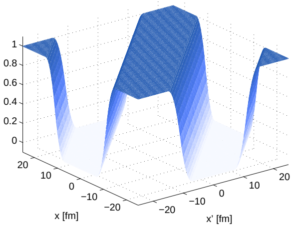

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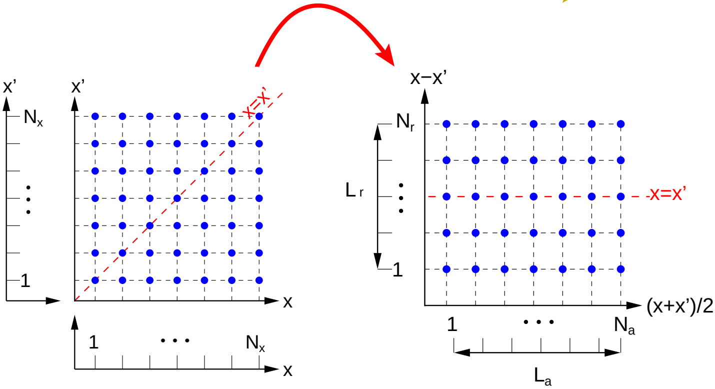
Off-diagonally filtered evolution

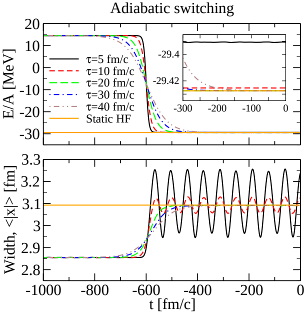
Rotated coordinate frame



- Traditional calculations performed on $N_x \times N_x$ mesh
- 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 $2 - 10$!

Traditional vs. rotated evolutions

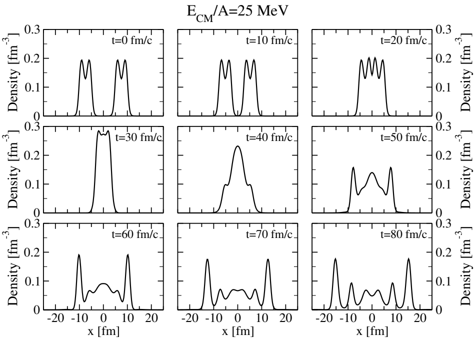
MF dynamics: summary



A. Rios *et al.*, Ann. Phys. **326**, 1274 (2011)

- Use adiabatic theorem to solve initial state ✓
- Phenomenology of 1D reactions ✓
- Full (N_x^2), damped & cut ($N_a \times N_r$) 1D mean-field evolution ✓
- Identified lack of correlations in Wigner distribution ✓

MF dynamics: summary



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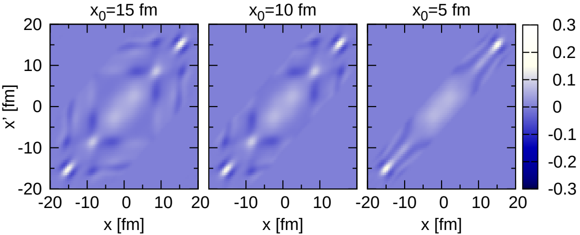
MF dynamics: summary

Off-diagonal elements



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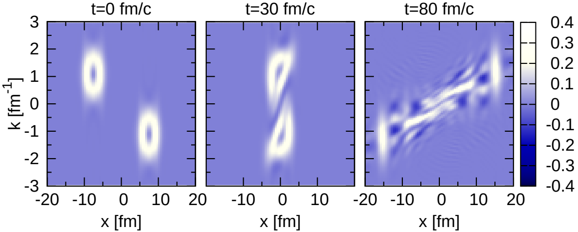
MF dynamics: summary

Wigner distribution



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Outline

Nuclear time-dependent correlations

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- Major goal: microscopic description of dissipation in 3D reactions

  - Thermalization $(0 < n_\alpha < 1)$
  - Damping of collective modes

$\Downarrow$

  - Improved description of fusion
  - Nuclear resonance widths

- Experience gathered in
  - Uniform nuclear systems

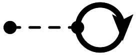
Wong & Tang, PRL **40**, 1070 (1978)
Danielewicz, Ann. Phys. **152**, 239 (1984)
H. S. Köhler, PRC **51**, 3232 (1995)

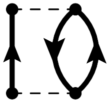
  - Nuclei

J. Aichelin & G. Bertsch, PRC **31**, 1730 (1985)
Tohyama, PRC **36**, 187 (1987)
C. Greiner & S. Leupold, Ann. Phys. **270**, 328 (1998)
W. Cassing *et al.*, Nucl. Phys. A **665**, 377 (2000)

Beyond mean-field time evolution

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





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

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

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

$$V(p) = V_0\sqrt{\pi}(\eta k)^2 e^{-\frac{(\eta k)^2}{4}} \Leftrightarrow V(x) = V_0\left(1 - 2\frac{x^2}{\eta^2}\right)e^{-\frac{x^2}{\eta^2}}$$

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UNIVERSITY OF SURREY

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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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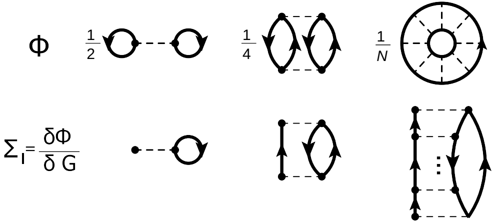

Puig von Friesen *et al.*, PRL **103**, 176404 (2009)

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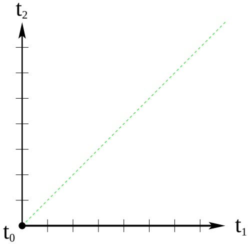
Two-time structure of equations

A challenging aspect

Mean-field time evolution



- TDHF mean-field propagation
  - Time diagonal: $\mathcal{G}(t_1, t_2) \rightarrow \mathcal{G}(t_1 = t_2 = t)$
  - Memory-less

- Kadanoff-Baym propagation (KABAB code)
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Köhler *et al*, Comp. Phys. Comm. **123**, 123 (1999)
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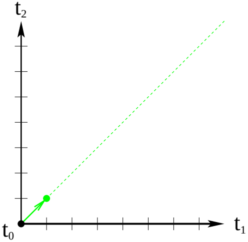

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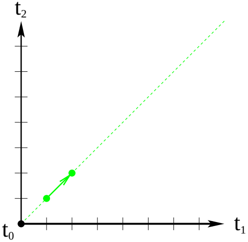

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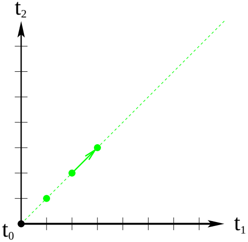

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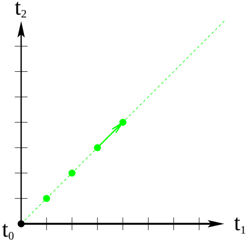

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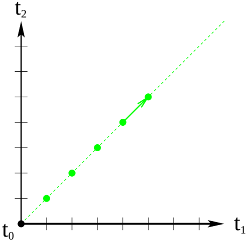

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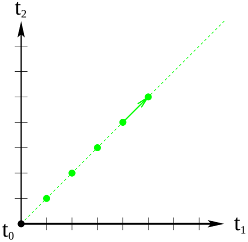
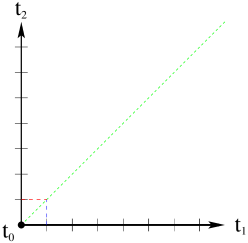


Correlated time evolution



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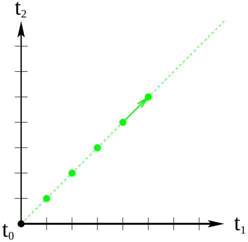

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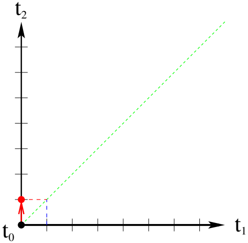

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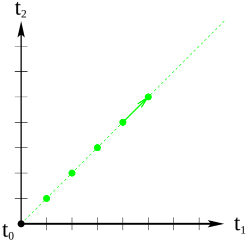

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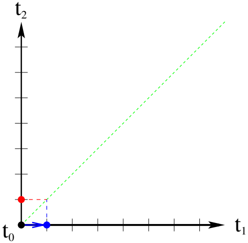

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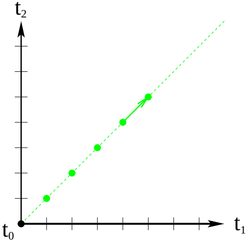

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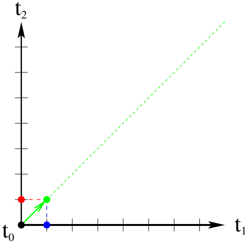

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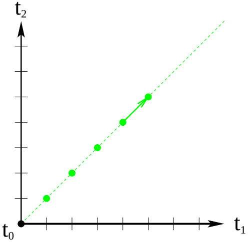

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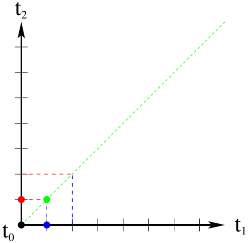

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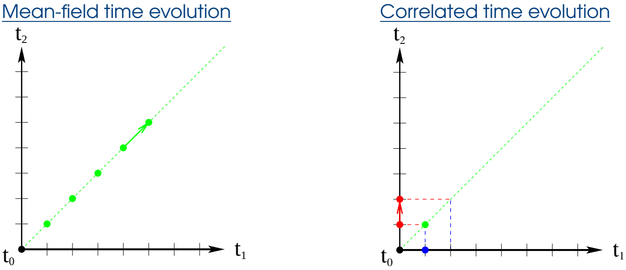
Stan, Dahlen & van Leeuwen, Jour. Chem. Phys. **130**, 224101 (2009)

Two-time structure of equations

A challenging aspect



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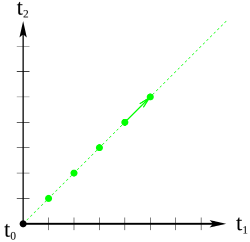
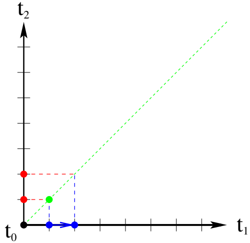


Correlated time evolution



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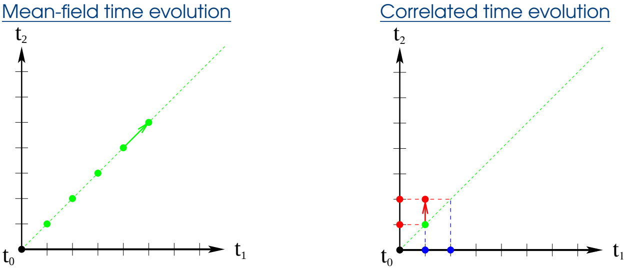

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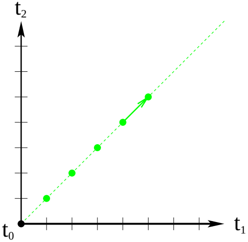

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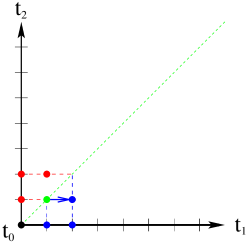

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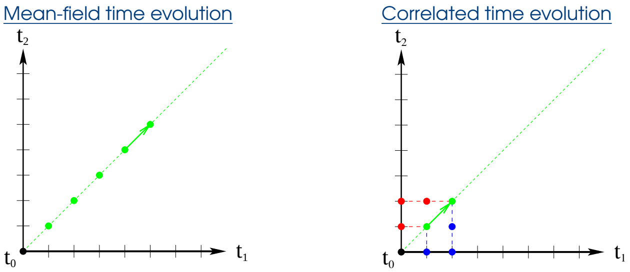

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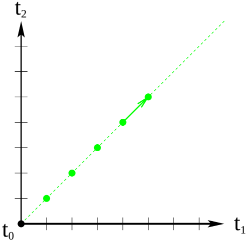

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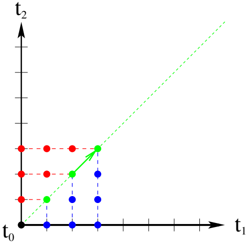

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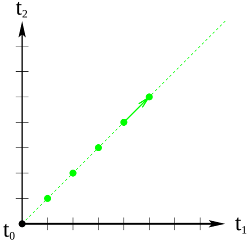

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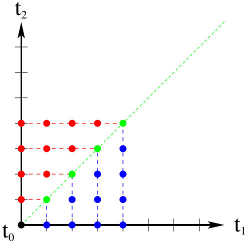

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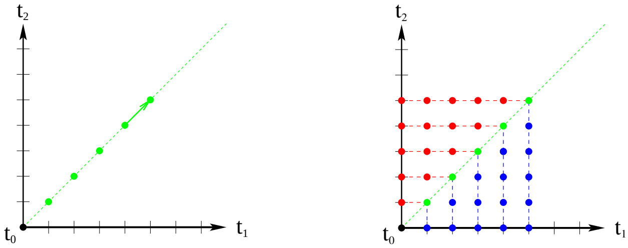

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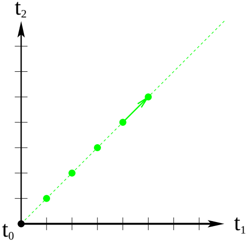

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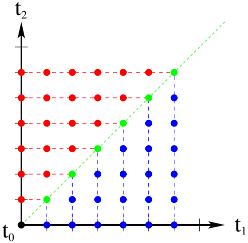

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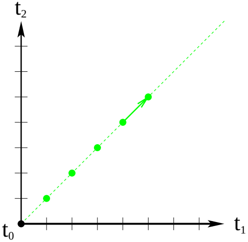

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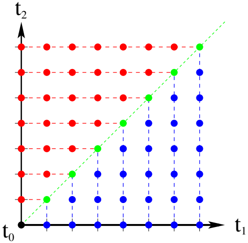

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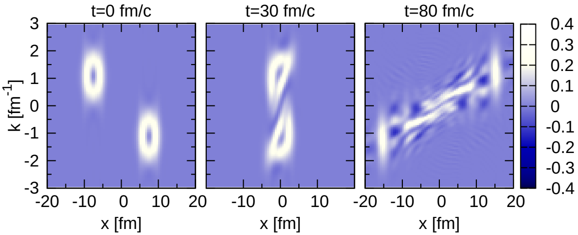
Correlated fermions in a trap

Correlated fermion in a trap: A=20

KB dynamics: summary

Wigner distribution



A. Rios *et al.*, Ann. Phys. **326**, 1274 (2011)

- Use adiabatic theorem to solve initial state ✓
- Phenomenology of 1D reactions ✓
- Full (N_x^2), damped & cut ($N_a \times N_r$) 1D mean-field evolution ✓
- Identified lack of correlations in Wigner distribution ✓
- Consistent 1D correlated evolution & memory issues
- Lessons learned ⇒ Progressive understanding of higher D

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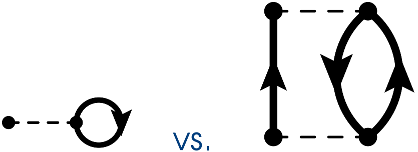

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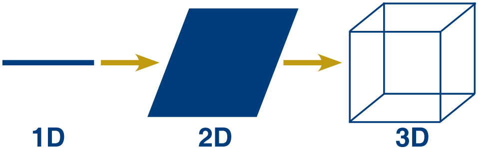

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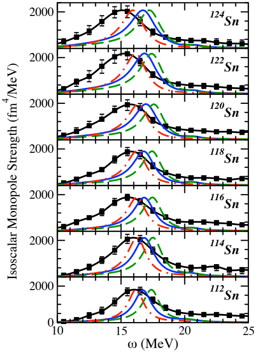
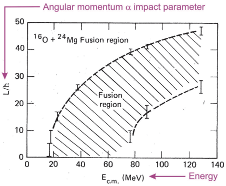
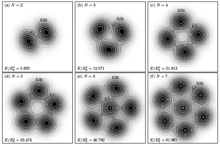
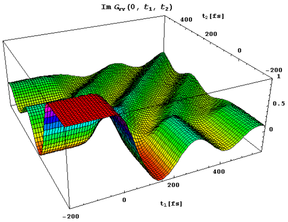
Nuclear Green's functions

Potential & challenges









- Potential for applications in nuclear reactions & structure
- Provide a microscopic understanding of dissipation
- Insight into bulk & transport properties of nuclei
- Work to be done on fluctuations
- Multidisciplinary research!

Thank you!