Dynamics of pair correlations

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"Solving the two-time Kadanoff-Baym equations..."
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Outline

Introduction

- Short-time Dynamics of many-body systems. 1-particle vs. 2-particle properties

How to access pair correlations

- Problems with Nonequilibrium Green's functions
- Pair correlations in single-time formalism

Initial correlations in the KB equations

Correlation dynamics using NEGF

Equilibrium pair correlations

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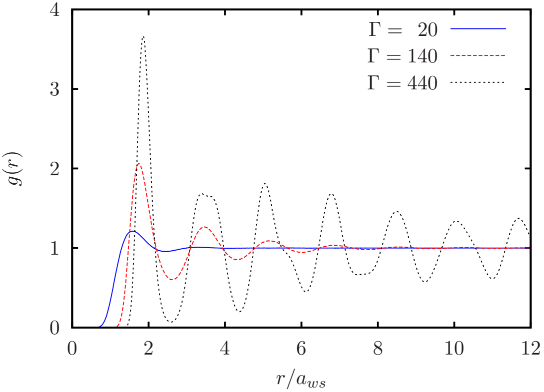
Stong Correlation effects: from ideal gas to crystal

Increasing correlation strength leads to increased particle localization (repulsive pair interaction).

Adequately reflected by pair distribution function.
Ideal system: $g(r) \equiv 1$.

Coupling parameter $\Gamma = \langle U \rangle / \langle K \rangle$



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Wigner crystallization in few-electron systems

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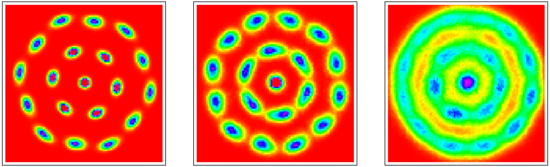
N Electrons in 2D quantum dot: (harmonic spherical confinement potential)

Density increase from left to right: orientational and radial melting



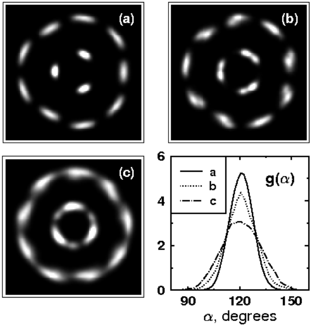
- First principle path integral Monte Carlo simulations

A. Filinov, MB and Yu.E. Lozovik, Phys. Rev. Lett. **86**, 3851 (2001)

Fluctuations captured by *angular pair distribution function* (right fig.)

- Extension to charged bosons: superfluidity, mesoscopic supersolid

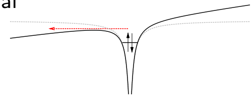
A. Filinov, J. Böning, MB, and Yu.E. Lozovik, Phys. Rev. B **77**, 214527 (2008)



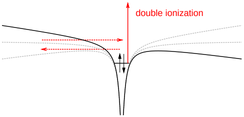
Photoionization processes in atoms. Correlation effects

- Example: Non-sequential double ionization of Helium
- double ionization increased by correlations. 1 electron theories (SAE) fail
- captured by time-dependent electron pair distribution function $g(\mathbf{r}_{12}, t)$

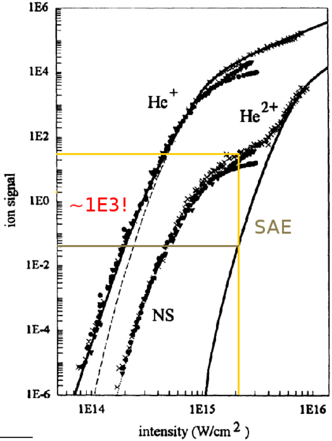
(1) one electron leaves binding potential



(2) field direction changes, electron accelerated towards the ion



(3) "kicks off" second electron



[1] B. Walker et al., Phys. Rev. Lett. **73**, 1227 (1994)

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Relevance of pair correlations

Two-particle correlations

- yield information about bound or scattering states: atoms, molecules, excitons etc.
- yield the static (and dynamic) structure factor
- identify relevant process (e.g. reaction channels)
- are experimentally measurable (coincidence methods), examples:
  - high energy collisions, fragmentation
  - chemical reaction products
  - "Reaction microscope" (COLTRIMS) electron-electron and electron-ion correlations with fs resolution
  - etc.

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Equations of motion for Keldysh Green function G

- Martin-Schwinger Hierarchy on Keldysh contour

$$[i\partial_t + h(1)]\; G(1,1') = \delta_c(1-1') \pm i \int_{\mathcal{C}} d2\; h^{\rm int}(1-2)\, G(12,1'2^+)$$

& adjoint

- Formal decoupling of hierarchy introducing selfenergy Σ

$$\pm i \int_{\mathcal{C}} d2\; h^{\rm int}(1-2)\, G(12,1'2^+) = \int_{\mathcal{C}} d2\, \Sigma(1,2)\, G(2,1')$$

beautiful results for single-particle Green's function, spectral function etc.

- But: loose easy access to pair correlations, contained in $G(12,12^+)$

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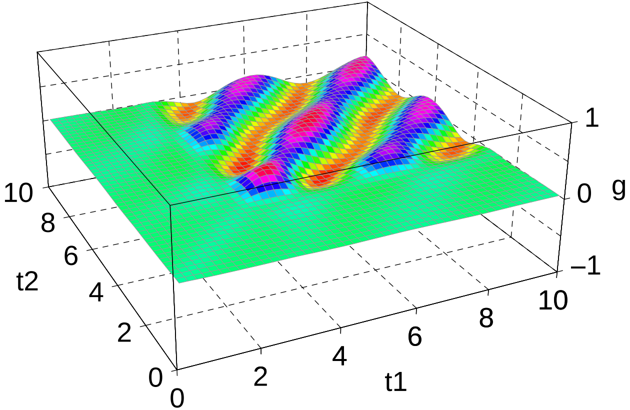
Evolution of two-time Green function



Build up of level population (along diagonal) and
of correlated spectrum (across diagonal, calculation by Karsten Balzer).

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How to obtain pair distributions from Keldysh Green function G

- Formal decoupling of hierarchy introducing selfenergy Σ

$$\pm i \int_{\mathcal{C}} d2\, h^{\rm int}(1-2)\, G(12, 1'2^+) = \int_{\mathcal{C}} d2\, \Sigma(1,2)\, G(2,1')$$

- two-time calculation yields $G(1,1')$ for given approximation $\Sigma[G]$
- **Solution 1**: Functional derivative

$$\pm G(12, 1'2^+) = \frac{\delta G(1,1')}{\delta v(2)} - i\langle \hat{n}(2)\rangle G(1,1')$$

  v: fictiteous single particle potential in $\hat{H}$ with $v \to 0$ at the end,

  or: real potential with scalar factor λ, $v \to \lambda v$: $dG(\lambda)/d\lambda|_{\lambda=1}$

  but: requires large (and dense) number of calculations for different v

- **Solution 2**: from known $\Sigma[G]$ reconstruct $G(12, 1'2')[G]$ dynamically (for each time step)

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Nonequilibrium BBGKY hierarchy

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Nonequilibrium Hierarchy of equations for reduced density operators (BBGKY)[1]

1-particle density operator $F_1(t) \sim \langle a^\dagger a \rangle \sim G^<(1,1')|_{t_1=t_1'=t}$

2-particle density operator $F_{12}(t) \sim \langle a^\dagger a^\dagger a a \rangle \sim G^<(1,2;1',2')|_{t_1=t_2=t_1'=t_2'=t}$

$$i\hbar\frac{\partial}{\partial t}F_1 - [H_1, F_1] = n\mathrm{Tr}_2[V_{12}, F_{12}], \tag{1}$$

$$i\hbar\frac{\partial}{\partial t}F_{12} - [H_{12}, F_{12}] = n\mathrm{Tr}_3[V_{13} + V_{23}, F_{123}], \tag{2}$$

$$i\hbar\frac{\partial}{\partial t}F_{123} - [H_{123}, F_{123}] = n\mathrm{Tr}_4[V_{14} + V_{24} + V_{34}, F_{1234}], \ldots \tag{3}$$

equal time limit of Martin-Schwinger hierarchy,
obtained from difference: MS-hierarchy minus adjoint ($\rightarrow$ commutators)

Transform second equation introducing pair *correlation* operator[2]:
$F_{12} = F_1(1)F_1(2) + c_{12}$

[1] for details see M. Bonitz *Quantum Kinetic Theory*
[2] for notational simplicity omit exchange (Fock) term

Evolution of pair correlation operator

$$i\hbar\frac{\partial}{\partial t}F_1 - [\bar{H}_1, F_1] = n\mathrm{Tr}_2[V_{12}, c_{12}] \tag{4}$$

$$i\hbar\frac{\partial}{\partial t}c_{12} - [\bar{H}_{12}, c_{12}] = [V_{12}, F_1F_2] + \tag{5}$$

$$n\mathrm{Tr}_3\Big\{[V_{13}, F_1c_{23}] + [V_{23}, F_2c_{13}] + [V_{13} + V_{23}, c_{123}]\Big\} \tag{6}$$

with mean field hamiltonians and Hartree potential U^H:

$$\bar{H}_1 = H_1 + U_1^H, \qquad U_1^H = n\mathrm{Tr}_2\, V_{12}\, F_2. \tag{7}$$

$$\bar{H}_{12} = \bar{H}_1 + \bar{H}_2 + V_{12}, \tag{8}$$

- known many-body approximations can be identified[3], e.g.
  - TD Hartree-Fock: $c_{12} \equiv 0$
  - 2nd Born approximation: $c_{123} = 0$ and neglect of ladder (V_{12} in H_{12}) and polarization diagrams [line (6)]
- numerical solution: coupled system for $F_1(t)$ and $c_{12}(t)$
  or: find analytical solution for $c_{12}(t)$ and insert into kinetic equation (4)[4]

[3] exists one to one correpondence to NEGF, including selfenergy

[4] avoided in NEGF by introducing selfenergy

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Evolution of pair correlation operator in Born approximation

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$$i\hbar\frac{\partial}{\partial t}F_1 - [\bar{H}_1, F_1] = n\mathrm{Tr}_2[V_{12}, c_{12}] \tag{9}$$

$$i\hbar\frac{\partial}{\partial t}c_{12} - [\bar{H}_1 + \bar{H}_1, c_{12}] = [V_{12}, F_1F_2] \tag{10}$$

with initial conditions (arbitrary): $F_1(t_0) = F_1^0$ and $c_{12}(t_0) = c^0$

Analytical solution for c_{12}:

$$c_{12}(t) = U_{12}^{0+}(tt_0)\, c^0\, U_{12}^{0-}(t_0t) + \tag{11}$$

$$+ \frac{1}{i\hbar}\int_{t_0}^{\infty} d\bar{t}\, U_{12}^{0+}(t\bar{t})\left\{\hat{V}_{12}F_1F_2 - F_1F_2\hat{V}_{12}^{\dagger}\right\}|_{\bar{t}}\, U_{12}^{0-}(\bar{t}t) \tag{12}$$

Free[5] propagator (retarded): $U_{12}^{0+}(tt') \longrightarrow \Theta(t-t')\, e^{-\frac{i}{\hbar}[\bar{E}_1^0+\bar{E}_2^0](t-t')}$

Initial correlation contribution [(11), decays] and correlation build up term (12)

Kinetic equation (9) contains two collision integrals (r.h.s): standard collision term involving (12) and additional integral with (11)[6].

[5] can be renormalized and damped, corresponds to $g^R(1,1')g^R(2,2')$

[6] Bonitz, Kremp, Phys. Lett. **212**, 83 (1996)

Evolution of pair correlation operator in Born approximation[7]

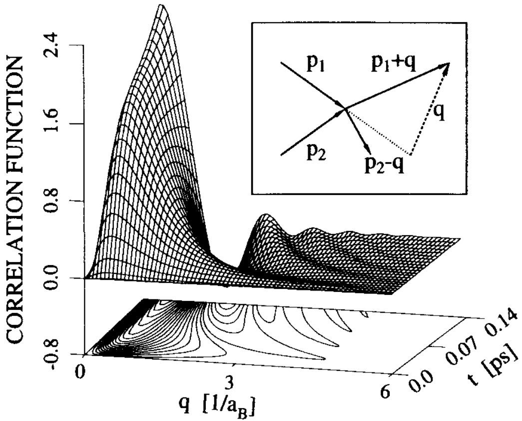

Figure: Imc_{12} for static e-e scattering in a homogeneous bulk semiconductor with $c_{12}^0 = 0$. $f^0(p)$ is a Gaussian centered at $k = 3a_B^{-1}$, $n = 3.64 \times 10^{17} cm^{-3}$. Initial momenta of the particle pair are $p_1 = p_2 = 3\hbar/a_B$ with $\mathbf{p}_1$ and $\mathbf{p}_2$ being parallel.

[7] from M. Bonitz, *Quantum Kinetic Theory*

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Initial correlations in the KB equations

- Martin Schwinger hierarchy defines initial value problem[8] for $G(1,1'), G(1,2,1',2')\dots$, need initial values at $t_1 = \dots t_2' = t_0$
- Early studies: Fujita, Hall, Craig, Tikhodeev, Danielewicz
- Special case of equilibrium initial correlations: solved by using deformed Keldysh contour (imaginary branch)
- Extension to general case:

$$I(1,1') = \pm i \int_{\mathcal{C}} d2\; V(1-2)\, G(12, 1'2^+) = \int_{\mathcal{C}} d2\, \Sigma(1,2)\, G(2,1')$$

valid for arbitrary t_1, t_1' on $\mathcal{C}$. In particular, for $t_1, t_1' \to t_0$:

$$I(t_0, t_0) = \pm i \int dr_2\; w(r_1 - r_2)\, G(12, 1'2^+)|_{t_0} = \lim_{t_1, t_1' \to t_0} \int_{\mathcal{C}} d2\, \Sigma(1,2)\, G(2,1')$$

only time-local selfenergies (such as Hartree-Fock) survive the limit

$\Rightarrow$ structure of $G(1,2,1',2')$ requires existence of additional selfenergy Σ^{IN}

[8] this is masked by the formal closure via the selfenergy

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Nonequilibrium initial correlations in the KB equations[9]

$$I(t_0,t_0) = \pm i \int dr_2\, w(r_1-r_2)\, G(12,1'2^+)|_{t_0} = \lim_{t_1,t_1'\to t_0} \int_{\mathcal{C}} d2\, \Sigma(1,2)\, G(2,1')$$
$$= \pm i \int dr_2\, w(r_1-r_2) \left\{ G^{HF}(12,1'2^+) + C(12,1'2') \right\} |_{t_0}$$

with 2-particle Hartree-Fock and correlation Green function (C):

$$G^{HF}(12,1'2') = G(1,1')G(2,2') \pm G(1,2')G(2,1')$$
$$C(12,1'2')|_{t_0} = c_{12}(t_0), \quad \text{1-time pair correlation operator}$$

- requires structure of selfenergy $\Sigma(1,1') = \Sigma^{HF} + \Sigma^{cor} + \Sigma^{IN}$

with $\Sigma^{HF}, \Sigma^{IN} \sim \delta_C(t_1 - t_1')$, Σ^{cor} does not contribute to $I(t_0,t_0)$

- Initial correlation selfenergy yields additional collision term:

$$I^{IN}(t_0,t_0) = \pm i \int dr_2\, w(r_1-r_2)\, c_{12}(t_0) = \lim_{t_1,t_1'\to t_0} \int_{\mathcal{C}} d2\, \Sigma^{IN}(1,2)\, G(2,1')$$

- Explicit results for Σ^{IN} in Born and T-matrix approximation available

[9] Semkat, Kremp, Bonitz, Phys. Rev. E **59**, 1557 (1999), J. Math. Phys. **41**, 7458 (2000)

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Example: 2nd Born approximation

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- spatially homogeneous system, momentum representation
- for $t = t' = t_0 : g^{R/A} = 1$
- initial correlation c evolves in time with free two-particle propagators

$$I^{\mathrm{IC}}(\mathbf{p}_1;t,t') = -2i\hbar^5\mathcal{V}\int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\frac{d\mathbf{q}}{(2\pi\hbar)^3}V(\mathbf{q})$$
$$\times g^{\mathrm{R}}(\mathbf{p}_1+\mathbf{q};t,t_0)g^{\mathrm{R}}(\mathbf{p}_2-\mathbf{q};t,t_0)\,c(\mathbf{p}_1+\mathbf{q},\mathbf{p}_2-\mathbf{q},\mathbf{p}_1,\mathbf{p}_2;t_0)\,g^{\mathrm{A}}(\mathbf{p}_2;t_0,t)g^{\mathrm{A}}(\mathbf{p}_1;t_0,t')$$

- same results as in 1-time approach (p. 15), except for full propagators
- examples for nonequilibrium initial correlations:
  - rapid quench (cooling)
  - rapid change of interaction potential[10]
  - rapid photoionization of atoms (switch of spin statistics)[11]
- unusual short-time relaxation possible: correlation induced cooling

[10] Gericke, Murillo, Semkat, Bonitz, Kremp, J. Phys. A: Math. Gen. **36**, 6087 (2003)
[11] Gericke, Murillo, Bonitz, Semkat, J. Phys. A: Math. Gen. **36**, 6095 (2003)

Effect of initial correlations on energy relaxation

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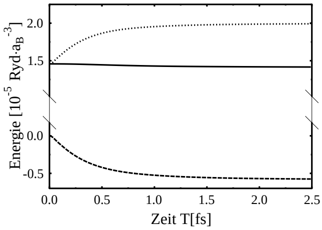
Dense hydrogen plasma, $T = 10,000K$, $n = 10^{21}cm^{-3}$, $k = 0.6/a_B$

Solution of KB equations conserves total energy $H(t) = T(t) + U(t) = H(0)$

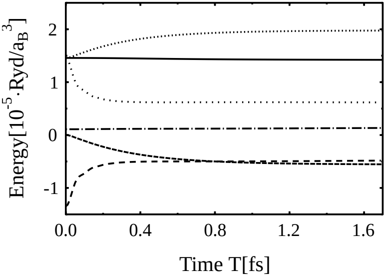
Initial state uncorrelated
(zero correlation energy U)

Correlations build up $\rightarrow$ increase of $|U|$
$\rightarrow$ Increase of kinetic energy T.



$T(t)$ and $U(t)$ saturate at correlation time $t \approx \tau_{cor} \sim \omega_{pl}^{-1}$

Uncorrelated vs. over-correlated initial state

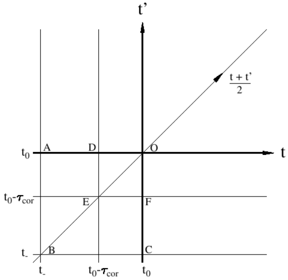


Preparing system in over-correlated initial state leads to cooling.

Semkat, Kremp, Bonitz, Phys. Rev. E **59**, 1557 (1999)
Bonitz/Semkat, *Introduction to Computational Methods for Many Body Systems*,

Physically relevant initial correlations c_{12}^0

Consistency: Only those c_{12}^0 are relevant which can be produced by a dynamical evolution[12], e.g. by two-time solution from an earlier uncorrelated state at t_-:



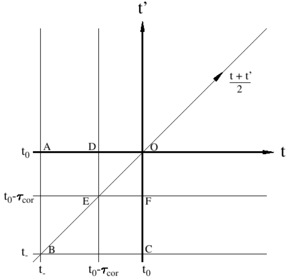
Example: Homogeneous system, collision terms in KBE at (t_0, t_0):

$$-2i\hbar\mathcal{V}\int\frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\frac{d\mathbf{q}}{(2\pi\hbar)^3}V(\mathbf{q})c(\mathbf{p}_1+\mathbf{q},\mathbf{p}_2-\mathbf{q},\mathbf{p}_1,\mathbf{p}_2;t_0)=$$

$$=\int_{t_-}^{t_0}d\bar{t}\left[\Sigma^>(\mathbf{p}_1;t_0,\bar{t})g^<(\mathbf{p}_1;\bar{t},t_0)-\Sigma^<(\mathbf{p}_1;t_0,\bar{t})g^>(\mathbf{p}_1;\bar{t},t_0)\right]$$

[12] Semkat, Bonitz, Kremp, Contrib. Plasma Phys. **43**, 321 (2003)

Semigroup property



If two-particle propagators possess semigroup property[13]

$$g_{12}^R(t, t_0) = g_{12}^R(t, t_1) g_{12}^R(t_1, t_0), \qquad t_0 \leq t_1 \leq t, \tag{13}$$

the time evolution can be continued in simple fashion, see below.

Yet this may be possible only in special cases. Otherwise there exists a more general semi-group property derived by Velicky et al., J. Phys. Conf. Ser. **35**, 1-16 (2006) [14]

[13] Semkat, Bonitz, Kremp, Contrib. Plasma Phys. **43**, 321 (2003)

[14] we thank Pawel Danielewicz for pointing this out to us

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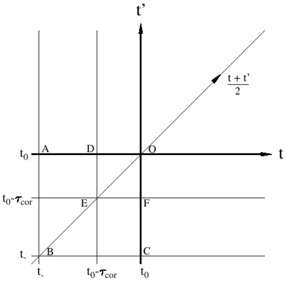
Semigroup property: Efficient continuation of calculations



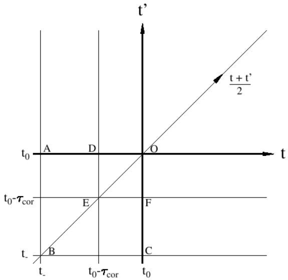
Advantage: (possibly substantial) reduction of 2-time simulation length,

Information from previous evolution (g, Σ) condensed in two lines $\overline{OA}$, $\overline{OC}$[15]

$$c(\mathbf{p}_1+\mathbf{q},\mathbf{p}_2-\mathbf{q},\mathbf{p}_1,\mathbf{p}_2;t_0) = \frac{i\hbar}{\mathcal{V}}\int_{t_-}^{t_0} d\bar{t}\, V(\mathbf{q})\left[g^>(\mathbf{p}_1+\mathbf{q},t_0,\bar{t})g^>(\mathbf{p}_2-\mathbf{q},t_0,\bar{t})g^<(\mathbf{p}_2;\bar{t},t_0)g^<(\mathbf{p}_1;\bar{t},t_0) - g^<(\mathbf{p}_1+\mathbf{q},t_0,\bar{t})g^<(\mathbf{p}_2-\mathbf{q},t_0,\bar{t})g^>(\mathbf{p}_2;\bar{t},t_0)g^>(\mathbf{p}_1;\bar{t},t_0)\right]. \quad (15)$$

[15] or even only $\overline{DO}$, $\overline{OF}$, if finite memory depth τ_{cor}

Propagation of initial (previous) correlations



Precomputed correlation c propgates for $t, t' \geq t_0$ via additional collision integral

$$I^{\mathrm{IC}}(\mathbf{p}_1;t,t') = -2i\hbar^5\mathcal{V}\int\frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\frac{d\mathbf{q}}{(2\pi\hbar)^3}V(\mathbf{q})$$

$$\times g^{\mathrm{R}}(\mathbf{p}_1+\mathbf{q};t,t_0)g^{\mathrm{R}}(\mathbf{p}_2-\mathbf{q};t,t_0)\,c(\mathbf{p}_1+\mathbf{q},\mathbf{p}_2-\mathbf{q},\mathbf{p}_1,\mathbf{p}_2;t_0)\,g^{\mathrm{A}}(\mathbf{p}_2;t_0,t)g^{\mathrm{A}}(\mathbf{p}_1;t_0,t')$$

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Dynamics of pair correlations with NEGF

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- Pair distribution h^{ab} of multi-component system:

$$h^{ab}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_2',t) \quad = \quad i^2 g^{ab,<}(1,2,1',2')|_{t_1=t_2=t_1'=t_2'=t}$$

- Follows from two-particle Green function g^{ab} on Keldysh contour
  g^{ab} obeys Bethe-Salpeter equation[16]:

$$g^{ab}(12,1'2') = g^a(1,1')g^b(2,2') \pm \delta_{ab} g^a(1,2')g^b(2,1') +$$
$$i\int_{\mathcal{C}} d\bar{1}d\bar{2}d\tilde{1}d\tilde{2}\, g^a(1,\bar{1})g^b(2,\bar{2})K^{ab}(\bar{1}\bar{2},\tilde{1}\tilde{2})\, g^{ab}(\tilde{1}\tilde{2},1'2')$$

Formal closure of second equation of MS hierarchy with interaction kernel K^{ab}

- Goal: compute h^{ab} from pre-computed single-particle Green function
- Problem: find K^{ab} for a given selfenergy Σ
- below: use Σ in Hartree-Fock plus 2nd Born approximation

[16] e.g. Bornath, Kremp, Schlanges, Phys. Rev. E (1999)

Two-particle kernel K^{ab} in Born approximation

1. Screened ladder approximation: $K^{ab}(\bar{1}\bar{2},\tilde{1}\tilde{2}) \to V^{ab}(\bar{1}\bar{2})\delta(\bar{t}_1-\tilde{t}_1)\delta(\bar{t}_2-\tilde{t}_2)$
2. Neglect dynamical screening: $V^{ab}(\bar{1}\bar{2}) \to V^{ab}(\bar{r}_{12})\delta(\bar{t}_1-\bar{t}_2)$, where $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$

$$g^{ab}(12,1'2') = g^a(1,1')g^b(2,2') \pm \delta_{ab}g^a(1,2')g^b(2,1')$$

$$+i\int_{\mathcal{C}} d\bar{t}\, g^a(1,\bar{1})g^b(2,\bar{2})V^{ab}(\bar{r}_{12})\, g^{ab}(\bar{1}\bar{2},1'2'), \quad \bar{t}_1=\bar{t}_2=\bar{t}$$

3. First iteration of integral equation (Born approximation):

$$\begin{aligned} g^{ab}(12,1'2') &= g^a(1,1')g^b(2,2') \pm \delta_{ab}g^a(1,2')g^b(2,1') \\ &+ i\int_{\mathcal{C}} d\bar{t}\, g^a(1,\bar{1})g^b(2,\bar{2})V^{ab}(\bar{r}_{12}) \\ &\times \left\{g^a(\bar{1},1')g^b(\bar{2},2') \pm \delta_{ab}g^a(\bar{1},2')g^b(\bar{2},1')\right\}, \\ &\text{with} \quad \bar{t}_1=\bar{t}_2=\bar{t}. \end{aligned}$$

4. need $g^{ab<}$ with four equal time arguments to compute pair distribution function. Note: g^{ab} has Keldysh matrix with 3^4 components!

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Single time two-particle Green function on Keldysh contour simpler:

$$g^{ab}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t) = g^{ab,HF}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t) + i\int_{\mathcal{C}} d\bar{t}\, G_0^{ab}(\mathbf{r}_1\mathbf{r}_2;\bar{\mathbf{r}}_1\bar{\mathbf{r}}_2,t\bar{t})\Sigma_0^{ab}(\bar{\mathbf{r}}_1\bar{\mathbf{r}}_2;\mathbf{r}_1'\mathbf{r}_2';\bar{t}t)$$

with defintion of ideal two-particle functions

$$G_0^{ab}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';tt') = g^a(\mathbf{r}_1t;\mathbf{r}_1't')g^b(\mathbf{r}_2t;\mathbf{r}_2't')$$

$$\Sigma_0^{ab}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';tt') = V^{ab}(r_{12})\left\{G_0^{ab}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';tt') \pm \delta_{ab}G_0^{ab}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_2'\mathbf{r}_1';tt')\right\}$$

Integral has same structure as collision integral in KBE

in case of equilibrium pair correlations: two contributions (beyond HF):

$$g_{cor}^{ab<} \sim G_0^{ab,<}\circ\Sigma_0^{ab,A} + G_0^{ab,R}\circ\Sigma_0^{ab,<}$$

$$g_{IC}^{ab<} \sim G_0^{ab,\rceil}\star\Sigma_0^{ab,\lceil}$$

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Result for pair correlations in Born approximation

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$$\frac{1}{i^2} h^{ab}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t) = \left\{ g^{abHF} + g^{ab<}_{cor} + g^{ab<}_{IC} \right\} (\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t)$$

$$i^2 g^{abHF}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t) = \rho^a(\mathbf{r}_1,t)\rho^b(\mathbf{r}_2,t) \pm \delta_{ab}\rho^a(\mathbf{r}_1\mathbf{r}_2,t)\rho^b(\mathbf{r}_2\mathbf{r}_1,t)$$

$$g^{ab<}_{cor}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t) = i\int_0^t d\bar{t}\int d^3\bar{r}_1 d^3\bar{r}_2 V^{ab}(\bar{r}_{12})\Big\{ g^{a,>}(\mathbf{r}_1 t;\bar{\mathbf{r}}_1\bar{t}) g^{b,>}(\mathbf{r}_2 t;\bar{\mathbf{r}}_2\bar{t}) \times$$

$$\left[g^{a,<}(\bar{\mathbf{r}}_1\bar{t},\mathbf{r}_1',t) g^{b,<}(\bar{\mathbf{r}}_2\bar{t},\mathbf{r}_2';t) \pm \delta_{ab} g^{a,<}(\bar{\mathbf{r}}_1\bar{t},\mathbf{r}_2',t) g^{b,<}(\bar{\mathbf{r}}_2\bar{t},\mathbf{r}_1';t)\right] - (> \leftrightarrow <)\Big\}$$

analogous result for $g^{ab<}_{IC}$ [17], agrees with one-time theory (p. 15)

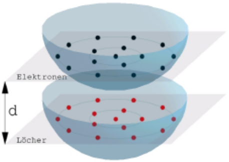
- Extract information on distance dependence:

Diagonal matrix elements: $\mathbf{r}_1 = \mathbf{r}_1'$, $\mathbf{r}_2 = \mathbf{r}_2'$
center of mass and relative coordinates: $\mathbf{R} = \frac{\mathbf{r}_1+\mathbf{r}_2}{2}$, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$
Result: local pair distribution $h^{ab}(\mathbf{r},\mathbf{R};t)$

[17] M. Bonitz, K. Balzer and L. Rosenthal, to be published

Equilibrium pair correlations in e-h bilayers[18]

- Spatially separated electrons and holes, $(N_e = N_h)$, masses $m^*_{e(h)}$
- zero thickness layers with distance d^*, harmonic in plane confinement
- coupling strength given by parameter λ



- Dimensionless Hamiltonian: $\left(\mathbf{r} \to \frac{\mathbf{r}}{r_0},\ r_0 = \sqrt{\frac{\hbar}{m_e^* \Omega}},\ \lambda = \frac{r_0}{a_B} \sim \sqrt{\frac{m_e^*}{\Omega}}\right)$

$$\hat{H}_e = \sum_{i=1}^{N_e} \frac{1}{2}\left(-\Delta_{i,e} + \mathbf{r}_{i,e}^2\right) + \lambda \sum_{i<j=2}^{N_e} \frac{1}{\sqrt{(\mathbf{r}_{i,e} - \mathbf{r}_{j,e})^2}}$$

$$\hat{H}_h = \sum_{i=1}^{N_h} \frac{1}{2}\left(-\frac{m_e^*}{m_h^*}\Delta_{i,h} + \frac{m_h^*}{m_e^*}\mathbf{r}_{i,h}^2\right) + \lambda \sum_{i<j=2}^{N_h} \frac{1}{\sqrt{(\mathbf{r}_{i,h} - \mathbf{r}_{j,h})^2}}$$

$$\hat{H}_{e-h} = -\lambda \sum_{i=1}^{N_e} \sum_{j=1}^{N_h} \frac{1}{\sqrt{(\mathbf{r}_{i,e} - \mathbf{r}_{j,h})^2 + d^{*2}}}$$

[18] Lasse Rosenthal, Diploma thesis, Kiel University 2009

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One-particle densities for weak and strong coupling

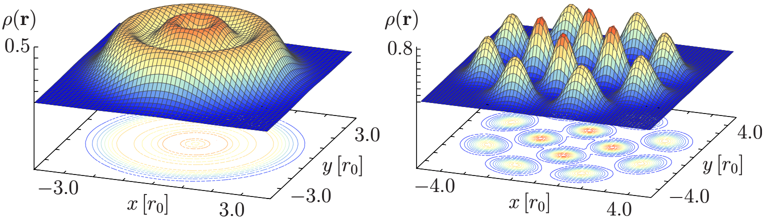

Figure: One-particle density for $N_{e(h)} = 12$ electrons and holes for $\lambda = 2.0$ (left figure) and $\lambda = 15.0$ (right figure)

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Equilibrium radial distribution functions

Calculation of the equilibrium pair correlation function in Hartree-Fock approximation:

- local pair distribution function:

$$h^{ab}_{HF}(\mathbf{R},\mathbf{r}) = g^{a}_{HF}(\mathbf{r}_1,\mathbf{r}_1)g^{b}_{HF}(\mathbf{r}_2,\mathbf{r}_2) - \delta_{ab}\, g^{a}_{HF}(\mathbf{r}_1,\mathbf{r}_2)g^{b}_{HF}(\mathbf{r}_2,\mathbf{r}_1)\big|_{\mathbf{r}_1=\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{r}_2=\mathbf{R}-\frac{\mathbf{r}}{2}}$$

- global pair distribution function:

$$h^{ab}_{HF}(\mathbf{r}) = \int d\mathbf{R}\, h^{ab}_{HF}(\mathbf{R},\mathbf{r})$$

- radial pair distribution function:

$$h^{ab}_{HF}(\mathbf{r}) \xrightarrow[\text{transformation}]{\text{coordinate}} h^{ab}_{HF}(r,\varphi)$$

$$h^{ab}_{HF}(r) = \int d\varphi\, r\, h^{ab}_{HF}(r,\varphi)$$

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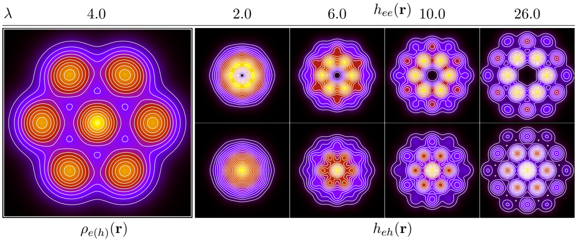
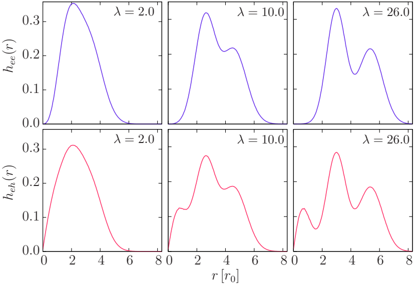
Results for radial pair distributions in e-h bilayers





- global pair distribution function for $N_{e(h)} = 7$ (upper figure)
- radial pair distribution function for $N_{e(h)} = 7$ (left figure)

$\longrightarrow$ different regimes of localisation

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Nonequilibrium pair correlations: computational aspects

$$\frac{1}{i^2} h^{ab}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t) \quad = \quad \left\{g^{abHF} + g^{ab<}_{cor} + g^{ab<}_{IC}\right\}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t)$$

$$g^{ab<}_{cor}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t) = i\int_0^t d\bar{t}\int d^3\bar{r}_1 d^3\bar{r}_2 V^{ab}(\bar{r}_{12})\Big\{g^{a,>}(\mathbf{r}_1 t;\bar{\mathbf{r}}_1\bar{t})g^{b,>}(\mathbf{r}_2 t;\bar{\mathbf{r}}_2\bar{t})\times$$

$$\left[g^{a,<}(\bar{\mathbf{r}}_1\bar{t},\mathbf{r}_1',t)g^{b,<}(\bar{\mathbf{r}}_2\bar{t},\mathbf{r}_2';t) \pm \delta_{ab}g^{a,<}(\bar{\mathbf{r}}_1\bar{t},\mathbf{r}_2',t)g^{b,<}(\bar{\mathbf{r}}_2\bar{t},\mathbf{r}_1';t)\right] - (>\leftrightarrow<)\Big\}$$

• Structure very similar to collision integral (obviously):

$$\pm i\int_{\mathcal{C}} d2\; V(1-2)\, G(12,1'2^+) = \int_{\mathcal{C}} d2\, \Sigma(1,2)\, G(2,1')$$

$\Rightarrow$ advantageous to compute on the fly, with the collision integral

• besides spatial correlations also correlations of various orbitals of interest: such as $h^{ab}_{kk,ll}$

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Conclusion & Outlook

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1. Pair correlations are key quantities for many-particle effects
2. Simple access in single-time theory (density operators): initial correlation term (decays) plus correlation build up
3. NEGF: nonequilibrium initial correlations give rise to additional selfenergy and collision integral
4. If pair propgators possess semi-group property: efficient restart of calculations possible, using nonequilibrium initial correlations
5. Explicit result for time-dependent pair correlations in Born approximation derived. Can be straightforwardly computed on the fly
6. Equilibrium pair correlations: first numerical results presented for strongly correlated electron-hole bilayer