Quantum Kinetic Theory for Artificial Atoms

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Carrier-carrier scattering and optical dephasing in highly excited semiconductors

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A quantitative analysis of carrier-carrier scattering and optical dephasing in semiconductors is presented and results are given for quasiequilibrium situations and for the relaxation of a kinetic hole in a quasithermal carrier distribution. The calculations involve direct numerical integration of the Boltzmann equation for carrier-carrier scattering in the Born approximation. The screening of the Coulomb interaction is treated consistently in the fully dynamical random-phase approximation. Carrier relaxation rates are extracted from the Boltzmann-equation solution and a quantitative test of the relaxation-time approximation for situations near thermal quasiequilibrium is performed. The parametric dependence of carrier-collision rates and dephasing on plasma density, temperature, and electron and hole masses is discussed and analyzed in terms of phase-space blocking and screening.

Lenard-Balescu collision integral, Phys. of Fluids 3, 52 (1960)

dynamically screened Coulomb potential

\[ W(q, \omega) = \frac{V(q)}{1 - V(q) P(q, \omega)} = V(q) \epsilon^{-1}(q, \omega) \]

unscreened potential \[ V(q) = \frac{4 \pi e^2}{Vq^2} \]

\[ P(q, \omega) = \lim_{\delta \to 0} 2 \sum_{\alpha, k} \frac{f_\alpha(k) - f_\alpha(|q + k|)}{\epsilon_\alpha(k) - \epsilon_\alpha(|q + k|) + i\hbar \omega + i\delta} \]
Outline

Introduction
- Artificial atoms
- Femtosecond relaxation processes
- Limitations of Boltzmann-type kinetic equations

Basics of Nonequilibrium Green’s Functions
- Second quantization
- Definition of Nonequilibrium Green’s functions (NEGFs)
- Equations of motion for the NEGF

Numerical Results. Applications
- Homogenous Coulomb systems. Plasmas
- Dynamics of charged particles in a trap

Conclusions
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Simulation: \( N = 2, 3, \ldots, 6 \) fermions in a 2D parabolical trap.
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Femtosecond relaxation processes

- **Femtosecond laser excitation of matter**
  - coherent semiconductor optics
  - time resolved relaxation dynamics of solids
  - fs dynamics of atoms and molecules

- **Interaction of high intensity lasers, free electron lasers with matter**
  - strong nonlinear excitation
  - correlation effects on fs and sub-fs time scale

- **Need: Nonequilibrium many-body theory**
  ⇒ selfconsistent treatment of correlations, quantum and spin effects
  Neccesary to go beyond standard Boltzmann kinetic equations
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  Equations of motion for the NEGF

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Limitations of Boltzmann-type kinetic equations

\[
\left\{ \frac{\partial}{\partial t} + \frac{\partial E}{\partial p} \frac{\partial}{\partial R} - \frac{\partial E}{\partial R} \frac{\partial}{\partial p} \right\} f(p, R, t) = I(p, R, t) \tag{1}
\]

\[I(p_1, t) = \frac{2}{\hbar} \int \frac{dp_2}{(2\pi\hbar)^3} \frac{d\tilde{p}_1}{(2\pi\hbar)^3} \frac{d\tilde{p}_2}{(2\pi\hbar)^3} \left| \frac{V(p_1 - \tilde{p}_1)}{e^{RPA}(p_1 - \tilde{p}_1, E(p_1) - E(\tilde{p}_1))} \right|^2 \]

\[\times (2\pi\hbar)^3 \delta(p_1 + p_2 - \tilde{p}_1 - \tilde{p}_2) \cdot 2\pi \delta(E_1 + E_2 - \tilde{E}_1 - \tilde{E}_2) \times \left\{ \tilde{f}_1 \tilde{f}_2 (1 \pm f_1)(1 \pm f_2) - f_1 f_2 (1 \pm \tilde{f}_1)(1 \pm \tilde{f}_2) \right\} |t|
\]

with quasiparticle energy \( E_i = E(p_i), \tilde{E}_i = E(\tilde{p}_i), f_i = f(p_i), \tilde{f}_i = f(\tilde{p}_i) \)

Example: Quantum Lenard-Balescu collision integral (Coulomb scattering)

Properties of Equation (1):

1. Conservation of kinetic energy, \( \frac{d}{dt} \langle E \rangle(t) = 0 \)
2. Equilibrium solution: \( f(p, t) \rightarrow \) Bose/Fermi/Maxwell distribution \( \rightarrow \) thermodynamic and transport properties of ideal gas
3. Eq. (1) limited to times larger than correlation time, \( t \gg \tau_{corr} \)

Properties (1)–(3) in conflict with present goal \( \Rightarrow \) Generalizations necessary
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Hamiltonian in second quantization

▶ **Hamiltonian for interacting system**

\[
H(t) = \int dq \, \psi^\dagger(q) \, h^0(q, t) \, \psi(q) + \frac{1}{2} \int dq \, d\bar{q} \, \psi^\dagger(q) \, \psi^\dagger(\bar{q}) \, h^{\text{int}}(q, \bar{q}) \, \psi(\bar{q}) \, \psi(q)
\]

e.g. \( h^0(x, t) = (p - eA(x, t))^2 + \Phi(x, t) \), \( h^{\text{int}}(x, \bar{x}) = \frac{e^2}{|x-\bar{x}|} \)

▶ **Field operators** \( \psi, \psi^\dagger \) with

- commutation relation for bosons (-),
- anti-commutation for fermions (+)

\[
\begin{align*}
\left[ \psi^\dagger(q), \psi^\dagger(q) \right]_\mp &= 0 \\
\left[ \psi(q), \psi^\dagger(\bar{q}) \right]_\mp &= \delta(q - \bar{q})
\end{align*}
\]

▶ ⇒ **Theory has “built in” spin statistics**

▶ **Symmetry/anti-symmetry of**

\( N \)–particle states exactly guaranteed
Macroscopic Observables

- **Equilibrium ensemble average.** Density operator

\[ \langle O \rangle = \text{Tr}(\hat{\rho}O), \quad \hat{\rho} = \frac{1}{Z} \exp(-\beta H - \mu N) \]

- **Nonequilibrium expectation values.** Switch on perturbing field at \( t = t_0 \)

\[ \langle O \rangle \rightarrow \langle O \rangle(t) \], use Heisenberg operators

\[
\langle O_H(t) \rangle = \frac{\text{Tr}(e^{\beta \mu N} U(t_0 - i\beta, t_0) U(t_0, t) O(t) U(t, t_0))}{\text{Tr}(e^{\beta \mu N} U(t_0 - i\beta, t_0))}
\]

- **with evolution operator** \((\hbar = 1)\)

\[ U(t, t_0) = \exp \left( -i \int_{t_0}^{t} d\bar{t} H(\bar{t}) \right) \]

\[ e^{-\beta H} \equiv U(t_0 - i\beta, t_0) \]

- **Time evolution runs along**

Keldysh-contour \( C \) [L.V. Keldysh, Sov. Phys. JETP, 20, 1018 (1965)]

\[ C = \{ t \in \mathbb{C} | \Re t \in [t_0, \infty], \Im t \in [t_0, -\beta] \} \]
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Definition of Nonequilibrium Green’s functions

- **One-particle Green function**
  \[ G(x\tilde{t}, x'\tilde{t}') = \pm \frac{1}{i} \left\langle T_{C} \left( \Psi^{\dagger}(x\tilde{t}) \Psi(x'\tilde{t}') \right) \right\rangle \]
  
  \(\tilde{t}, \tilde{t}'\) belong to one of 3 branches, \(G\) is \(3 \times 3\) matrix

- **Keldysh Green functions** (matrix elements on \(C\)), denote \(1 \equiv r_1, t_1, s_{z1}\)

- **retarded/advanced functions**
  \[ g^{R/A}(1, 1') = \pm \Theta[\pm(t_1 - t'_1)] \left\{ g^> - g^< \right\} \]

- **real branch - imaginary branch components**
  \[ g^{R}(1, 1'), g^{A}(1, 1') \]

- **imaginary branch component**: Matsubara (equilibrium) GF
  \[ g^{M}(1, 1') \]
Physical content: Time-dependent macroscopic observables

\[ \langle \hat{O}(t) \rangle = \int dx \left[ o(x', t) \langle \Psi^\dagger (x t) \Psi (x' t) \rangle \right]_{x=x'}, \]

\[ = \mp i \int dx \left[ o(x', t) g^<(x t, x' t) \right]_{x=x'} \]

Particle density:

\[ \langle \hat{n}(x, t) \rangle = \langle \hat{n}(1) \rangle = \mp i g^<(1, 1) \]

Density matrix:

\[ F(x_1, x'_1, t) = \mp i g^<(1, 1') \big|_{t_1=t'_1} \]

Current density:

\[ \langle \hat{j}(1) \rangle = \mp i \left[ \left( \frac{\nabla_1}{2i} - \frac{\nabla_{1'}}{2i} + A(1) \right) g^<(1, 1') \right]_{1'=1} \]

Interaction energy, also follows from 1-particle function, [Baym/Kadanoff]

\[ \langle V(t) \rangle = \pm i \frac{V}{4} \int \frac{dp}{(2\pi \hbar)^3} \left\{ (i \partial_t - i \partial_{t'}) - \frac{p^2}{m} \right\} g^<(p, t, t') \big|_{t=t'} \]
Nonequilibrium Green's Functions

Definition and properties of NEGFs

- **Wigner distribution**
  \[ f(p, R, T) = \pm i \int d\omega \, g^<(RT, p\omega) \]

- **CoM and relative variables**
  \[ T = \frac{(t_1 + t_2)}{2}, \quad t = t_1 - t_2 \]
  \[ R = \frac{(x_1 + x_2)}{2}, \quad r = x_1 - x_2 \]

- **Single particle spectrum (Spectral function)**
  \[ a(\omega; R, p, T) = i \int dt \, e^{i\omega t} \left[ g^> - g^< \right] \left( T + \frac{t}{2}, T - \frac{t}{2}, R, p \right) \]

- **Nonequilibrium Density of states,** \[ \rho(\omega) = \text{Tr}(a(\omega; R, p, T)) \]

- **Example: Electrons in harmonic oscillator potential** \[ V \]

\[ \rho(\omega) \]

\[ V(x) \]

\[ \text{ideal} \]

\[ \text{corr} \]

\[ \epsilon_0, \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4 \]

\[ \omega \]

\[ \text{Im} \, g^<(t_1, t_2) \]

\[ t_2 \]

\[ t_1 \]
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Equations of motion for Keldysh Green function $G$

- **Heisenberg’s equation of motion:**
  \[ i \partial_t \Psi^{(\dagger)}(q, t) = \left[ \Psi^{(\dagger)}(q, t), H(t) \right] \]

- **Result:** **Martin-Schwinger Hierarchy** for one, two ... s-particle Green functions
  \[
  (i\partial_t + h(1)) \, G(1, 1') = \delta(1 - 1') \pm i \int_C d2 \, h^{\text{int}}(1 - 2) \, G(12, 12^+) \quad \& \quad \text{adjoint}
  \]

- **Formal decoupling of hierarchy** introducing **selfenergy** $\Sigma$
  \[
  \pm i \int_C d2 \, h^{\text{int}}(1 - 2) \, G(12, 12^+) = \int_C d2 \, \Sigma(1, 2) \, G(2, 1')
  \]

- **Conserving approximations**
  \[
  \Sigma[G](1, 2) = \frac{\delta \Phi[G]}{\delta G(2, 1)}
  \]
  

- **Example for $\Sigma$:** 1st and 2nd order diagrams $\Rightarrow$ Hartree-Fock + Second Born.
Keldysh-Kadanoff-Baym equations for matrix components* of $G$

\[
(i\partial_t - h(1)) g^\triangleright (1, 2) = \left[ \Sigma^R \circ g^\triangleright + \Sigma^\triangleright \circ g^A + \Sigma^\downarrow \star g^\uparrow \right] (1, 2)
\]

\[
(-i\partial_t - h(2)) g^\triangleright (1, 2) = \left[ g^R \circ \Sigma^\triangleright + g^\triangleright \circ \Sigma^A + g^\downarrow \star \Sigma^\uparrow \right] (1, 2)
\]

\[
(i\partial_t - h(1)) g^\downarrow (1, 2) = \left[ \Sigma^R \circ g^\downarrow + \Sigma^\downarrow \star g^M \right] (1, 2)
\]

\[
(-i\partial_t - h(2)) g^\downarrow (1, 2) = \left[ g^\downarrow \circ \Sigma^A + g^M \star \Sigma^\uparrow \right] (1, 2)
\]

\[
(-\partial_\tau - h(1)) g^M (1, 2) = i\delta(\tau - \tau') + \left[ \Sigma^M \star g^M \right] (1, 2)
\]

\[
(\partial_\tau - h(2)) g^M (1, 2) = i\delta(\tau - \tau') + \left[ \Sigma^M \star g^M \right] (1, 2)
\]

* matrix algebra: DuBois, Langreth, ..., Short notation:

\[
[A \circ B](12) = \int_{t_0}^{\infty} d\bar{\tau} d\bar{x} A(1, \bar{x}\bar{\tau}) B(\bar{x}\bar{\tau}, 2), \quad [A \star B](12) = -i \int_0^\beta d\bar{\tau} d\bar{x} A(1, \bar{x}\bar{\tau}) B(\bar{x}\bar{\tau}, 2)
\]

**Equilibrium initial state**: $g(t_0, t_0)$
- defined by precomputed $g^M$

**Nonequilibrium initial state**: $g(t_0, t_0)$
- given by $f(t_0)$, initial pair correlations $c_{12}(t_0)$, additional selfenergy $\Sigma^{IC}$

[Ref: Danielewicz, Kremp/Semkat/Bonitz]
Numerical solution of Keldysh-Kadanoff-Baym Equations.

- **Full two-time solutions**: Danielewicz, Schäfer, Köhler/Kwong, Bonitz/Semkat, Haug, Jahnke, van Leeuwen ...

- **Equilibrium initial conditions**
  \[ g^< (0, 0) = i g^M (0^+), \]
  \[ g^\dagger (0, -i\tau) = i g^M (-\tau), \]
  \[ g^\dagger (-i\tau, 0) = i g^M (\tau). \]

- **Numerical scheme**
  1. Choose proper basis set
  2. Solve equilibrium problem: Dyson equation \[ \rightarrow g^M (\tau) \]
  3. Time-propagation: Solve Keldysh-Kadanoff-Baym equations
  \[ \rightarrow g^< (t, t'), g^\dagger / [g (t, t')] \]
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Sub-femtosecond energy relaxation in dense plasma

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

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 \( t \approx \tau_{cor} \sim \omega_{pl}^{-1} \)

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

Solution of KKB equations for short monochromatic excitation, \( U(t) = U_0(t) \cos q_0 r \)

Periodic density fluctuation, with Landau plus correlation damping

Fourier transform yields dynamic structure factor \( S(q, \omega) \)

- Conservation properties of KBE guarantee exact sum rule preservation of plasmon spectrum \( S(q, \omega) \)
- Simple approximations for selfenergy (such as 2nd Born approximation) give high-level correlation effects, including vertex corrections, in \( S \)

[Keong/Bonitz, PRL 84, 1768 (2000)]
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Hamiltonian and system parameters. 1D model

\[ H = \int dx \, \hat{\Psi}^\dagger(x) \, h^0(x, t) \, \hat{\Psi}(x) + \frac{1}{2} \int dx_1 \, dx_2 \, \hat{\Psi}^\dagger(x_1) \, \hat{\Psi}^\dagger(x_2) \, w(x_1, x_2) \, \hat{\Psi}(x_2) \, \hat{\Psi}(x_1) \]

\[ h^0(x, t) = -\frac{\hbar^2 \nabla^2_x}{2m} + \frac{m}{2} \Omega^2 x^2 + V_{\text{ext}}(x, t), \quad w(x_1, x_2) = \lambda \frac{x_0 \hbar \Omega}{\sqrt{(x_1 - x_2)^2 + a^2}} \]

- Dipole field
  \[ V_{\text{ext}}(x, t) = -e \, E(t) \, x \]
  \[ E(t) = a_0 \, e^{-\frac{(t-t_0)^2}{2t_1}} \, \cos(\omega t) \]
  \( \omega, a_0 \): dimensionless laser frequency and amplitude

- Coupling parameter \( \lambda \), inverse temperature \( \beta \):
  \[ \lambda = \frac{e^2}{x_0 \, \hbar \Omega}, \quad x_0^2 = \frac{\hbar}{m \Omega}; \quad \beta = \hbar \Omega / kT \]

- Expand Green functions in oscillator basis, \( g \rightarrow g_{kl} \)
Equilibrium density $n(x)$ and energy distribution $f(\epsilon_k - \mu)$

$N = 6$ fermions (1D trap)
Energy evolution after laser excitation

\[ \varepsilon_0 = 0.8 \quad \omega = 1.4 \quad N = 3\]
\[ \beta = 3.0 \quad \lambda = 1.0 \]

\[ E_{\text{tot}} \quad E_{\text{single}} \quad E_{\text{pot}} \quad E_{\text{kin}} \quad E_{\text{HF}} \]

\[ \Delta E \]

\[ t \quad [\Omega^{-1}] \]
Occupation number dynamics for off-resonant laser excitation

\[ \varepsilon_0 = 2.2 \quad N = 3 \]
\[ \omega = 3.0 \quad \beta = 3.0 \]
\[ \lambda = 1.2 \]

Pulse [a.u.]

Occup. probability \( n_k(t) \)

time \( t [\Omega^{-1}] \)
Occupation number dynamics for near-resonant laser excitation

\[ \mathcal{E}_0 = 0.8 \quad \omega = 1.4 \quad N = 3 \quad \beta = 3.0 \quad \lambda = 1.0 \]

\[ n_k(t) \]

\[ \text{time } t [\Omega^{-1}] \]
Evolution of Green function of ground state

along diagonal: weak change of ground state population, across: renormalized ground state energy (w.r. to $\mu$)
Evolution of Green function of level 3

along diagonal: reduction of population of level 3
Evolution of Green function of level 5

Build up of population of level 5 (along diagonal) and of correlated spectrum (across)
Conclusions & Outlook

- fs and sub-fs radiation sources ⇒ ultrafast dynamical response of matter
- **Ultrafast dynamics of Coulomb correlations.** Correlation build up ⇒ requires non-Markovian kinetic treatment
- **Real-time nonequilibrium Green functions** (Keldysh/Kadanoff-Baym)
  - selfconsistent non-perturbative treatment of strong fields
  - total energy conservation, exact spin statistics
- **Numerical applications: propagation of NEGF in two-time plain**
  - semiconductors, dense plasmas, electron gas
  - dynamics of trapped electrons, excitons, Bose condensates
  - atoms, molecules in strong fields ⇒ GW approximation
  for larger/complex systems: nonequilibrium combinations with DFT, QMC

- **Text books, reviews:**
  - *Introduction to Computational Methods in Many Body Physics*, M. Bonitz and D. Semkat (eds.), 2006
  - M. Bonitz *Quantum Kinetic Theory*, 1998
- **Announcement:** Interdisciplinary conference *Progress in Nonequilibrium Green Functions IV*, August 17-22 2009, Glasgow, Scotland

- **Web page:** www.theo-physik.uni-kiel.de/~bonitz
Basis representation of Nonequilibrium Green’s Functions.

- With an arbitrary but orthonormal set \( \{ \phi_k(x) \} \):

\[
g^{\geq}(x_t, x'_t) = \sum_{kl} \phi_k^*(x) \phi_l(x) g^{\geq}_{kl}(t, t'), \quad \psi^\dagger(x, t) = \sum_k \phi_k^*(x) \hat{a}_k^\dagger(t)
\]

- Equations of motion (KKBE) → matrix equations of exactly same structure. But spatial degrees of freedom separated.

- Dyson equation for Matsubara (equilibrium) Green’s function.

\[
\left[ -\partial_\tau - H^0 \right] \circ g^M(\tau) = \delta(\tau) + \int_0^\beta d\bar{\tau} \Sigma[g^M](\tau - \bar{\tau}) \circ g^M(\bar{\tau})
\]

- Real-time stepping: Kadanoff-Baym equations.

\[
\begin{align*}
i \partial_t g^> (t, t') &= h^{HF+Ext}(t) \circ g^> (t, t') + l^> (t, t') \\
-i \partial_t g^< (t', t) &= g^< (t', t) \circ h^{HF+Ext}(t) + l^< (t', t) \\
i \partial_t g^\dagger (t, -i\tau) &= h^{HF+Ext}(t) \circ g^\dagger (t, -i\tau) + l^\dagger (t, -i\tau) \\
-i \partial_t g^\dagger (-i\tau, t) &= g^\dagger (-i\tau, t) \circ h^{HF+Ext}(t) + l^\dagger (-i\tau, t)
\end{align*}
\]