Kinetic theory of correlated quantum systems in the framework of Zubarev's Nonequilibrium Statistical Operator Method (NSOM)

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Outline

- **A brief account of Zubarev's NSOM**
- **Kinetic description of nonequilibrium correlated systems**
- **Examples of relevant long-lived correlations**
- **Unification of kinetics and hydrodynamics for correlated systems**
- **Some challenges**

- "Relevant observables" $\langle P_m \rangle^t \equiv \mathrm{Tr}\,(P_m \varrho(t))$
- The quantum Liouville equation with a boundary condition (Zubarev's NSOM)

$$\frac{\partial \varrho(t)}{\partial t} + \frac{1}{i\hbar}\left[\varrho(t), H\right] = -\varepsilon\left\{\varrho(t) - \varrho_{\rm rel}(t)\right\}, \quad \varepsilon \to +0$$

- The general form of the relevant statistical operator (It corresponds to the maximum of entropy with given values of $\langle P_m \rangle^t$:

$$\varrho_{\rm rel}(t) = Z^{-1}(t)\exp\left\{-\sum_m F_m(t) P_m\right\},$$

  where $F_m(t)$ are the Lagrange multipliers.
- The self-consistency conditions (nonequilibrium equations of state)

$$\langle P_m \rangle^t = \langle P_m \rangle^t_{\rm rel} \equiv \mathrm{Tr}\left\{P_m \varrho_{\rm rel}(t)\right\}$$

- Generalized transport equations for observables

$$\frac{\partial \langle P_m \rangle^t}{\partial t} = \langle \dot{P}_m \rangle^t_{\text{rel}} + \sum_n \int_{-\infty}^{t} \mathrm{e}^{-\varepsilon(t-t')} \, \mathcal{L}_{mn}(t,t') F_n(t') \, dt',$$

where $\dot{P}_m = [P_m, H]/i\hbar$, and $\mathcal{L}_{mn}(t,t')$ are the generalized "kinetic coefficients".

Comments:

1) Despite the formally simple structure, the generalized transport equations are in fact very complicated (projected evolution in $\mathcal{L}_{mn}(t,t')$ etc.).

2) Kinetic coefficients contain "memory" effects. The Markovian approximation is adequate only if the set of observables $\{\langle P_m \rangle^t\}$ describes all relevant long-lived correlations.

- The model Hamiltonian (for illustration): $H = H_0 + H'$

$$H_0 = \sum_{11'} h(1',1)\, a^\dagger_{1'} a_1 \quad H' = \frac{1}{2} \sum_{121'2'} V_2(1'2',12)\, a^\dagger_{2'} a^\dagger_{1'} a_1\, a_2,$$

where the label k denotes a complete set of single-particle quantum numbers.

- Kinetic description in terms of reduced density matrices:

$$f_s(1\dots s, 1'\dots s'; t) = \langle a^\dagger_{s'} \dots a^\dagger_{1'} a_1 \dots a_s \rangle^t, \quad s = 1, 2, \dots$$

- Hierarchy for the reduced density matrices

$$\frac{\partial}{\partial t} f_s(1\dots s, 1'\dots s'; t) - \frac{1}{i\hbar} \langle [\, a^\dagger_{s'} \dots a^\dagger_{1'} a_1 \dots a_s, H\,] \rangle^t$$

$$= -\varepsilon \left\{ f_s(1\dots s, 1'\dots s'; t) - \bar{f}_s(1\dots s, 1'\dots s'; t) \right\},$$

where $\quad \bar{f}_s(1\dots s, 1'\dots s'; t) = \mathrm{Tr}\left(\varrho_{\mathrm{rel}}(t)\, a^\dagger_{s'} \dots a^\dagger_{1'} a_1 \dots a_s\right).$

Comments:

1) For macroscopic systems, it is expected that all boundary conditions are equivalent if one deals with exact solutions of the hierarchy.

2) Similar approximations in the hierarchy lead to different kinetic equations for different boundary conditions.

3) The Markovian approximation is adequate only if $\varrho_{\mathrm{rel}}(t)$ describes all relevant long-lived correlations.

4) For example, complete weakening of initial correlations (Bogoliubov's boundary condition):

$$\varrho_{\mathrm{rel}}(t) = Z^{-1}(t) \exp\left\{-\lambda_1(1', 1; t)\, a^{\dagger}_{1'} a_1\right\}, \quad f_1(t) = \overline{f}_1(t)$$

Relevant correlations: $\bar{g}_2(t) = \overline{f}_2 - \overline{f}_1 \overline{f}_1 = 0$. **NB:** In this case nonequilibrium correlations manifest themselves through memory effects.

- “Cluster” correlations (e.g., binary correlations)

$$\varrho_{\rm rel}(t) = Z^{-1}(t)\exp\Big\{ -\lambda_1(1',1;t)a^{\dagger}_{1'}a_1 - \frac{1}{2}\lambda_2(1'2',12;t)\,a^{\dagger}_{2'}a^{\dagger}_{1'}a_1 a_2\Big\}$$

  Relevant correlations: $\bar{g}_2(t) = g_2(t)$.
  Applications: dense systems with bound states.

- “Hydrodynamic” correlations:

$$\varrho_{\rm rel}(t) = Z^{-1}(t)\exp\Big\{ -\lambda_1(1',1;t)a^{\dagger}_{1'}a_1 - \int d\boldsymbol{r}\,\beta(\boldsymbol{r},t)H(\boldsymbol{r})\Big\}$$

  Relevant correlations: $\bar{g}_2(t) = \bar{g}_2[\beta(t),\lambda_1(t)]$; $\beta(\boldsymbol{r},t)$ plays the role of “inverse quasi-temperature”.

Physical arguments:

- The energy conservation implies that $\langle H(\boldsymbol{r})\rangle^t$ is a “slow varying quantity” on the kinetic and hydrodynamic time scales.
- The average $\langle H(\boldsymbol{r})\rangle^t$ is not determined completely by $f_1(t)$, so that the energy density must be treated as an independent relevant observable.

- Bogoliubov's boundary condition (weak interaction or low density)

  Markovian Boltzmann-type kinetic equations for $f_1(t)$. Correlations are included through memory effects (the so-called "Levinson kinetic equations"). Problems with energy conservation and the equilibrium solution.

- "Cluster" correlations

  A Markovian kinetic equation for f_1 coupled with a relaxation equation for "cluster" correlation functions, e.g., for $g_2(t)$. Correct conservation laws and equilibrium solutions. Problems with approximations in the transport equations (to ensure the energy conservation!).

- "Hydrodynamic" correlations

  A Markovian kinetic equation for $f_1(t)$ coupled with hydrodynamic equations. Cross-sections in the kinetic equation depend on $\bar{g}_2$. Correct conservation laws and equilibrium solutions.

- Conservation laws account for nonequilibrium long-lived many-particle correlations. The energy conservation is of special importance because the density of the interaction energy is determined by $f_2(t)$ (not by $f_1(t)$). Thus, strictly speaking, kinetic processes must always be treated together with the evolution of locally conserved quantities, i.e., with hydrodynamic processes.

Literature:

- Classical gases. The Bogoliubov (BBGKY) hierarchy with modified boundary conditions

  Zubarev D.N., Morozov V.G., Teor. Mat. Fiz. **60**, 270 (1984)

  Theoret. and Math. Phys. **60**, 814 (1984) (Eng. transl.)

  The Markovian binary collision approximation leads to the Enskog-type kinetic equation (instead of the Boltsmann equation)

- Dense quantum systems. Inclusion the mean energy into the set of relevant variables

  Morozov V.G. and Röpke G., Physica A **221**, 511 (1995)

  Quantum generalization of the Enskog approach. Collision integrals include the two-particle correlation matrix $\bar{g}_2$. The kinetic equation conserves the total energy.

- Correlation contributions in non-Markovian kinetic equations

  Morozov V.G. and Röpke G., J. Stat. Phys. **102**, 285 (2001)

  Nonequilibrium "hydrodynamic" correlations contribute to non-Markovian kinetic equations even in the Born approximation (weak interaction). It is precisely the interplay between collisions and correlations that is responsible for the correct behavior of non-Markovian collision integrals (e.g., the energy conservation and cancellation between the "collision" and "correlation" contributions in equilibrium).

Some challenges

- Inclusion of nonequilibrium “cluster” and/or “hydrodynamic” correlations in the Green’s function method
  The “Mixed” Green’s function approach to quantum kinetics with initial correlations:
  Morozov V.G., Röpke G., Ann. Phys. **278**, 127 (1999)
- Nonequilibrium correlations in relativistic kinetics
  At the moment the relativistic kinetic theory does not go beyond the quasiparticle picture.
- Application of the Enskog-type quantum kinetic equations to heavy-ion collisions
  An attractive feature of the Enskog-type equations: an interpolation approach applicable to the transition
  (Fermi liquid) $\rightarrow$ (semi-quantum dense hot matter) $\rightarrow$
  (a low density gas).