Fluctuations due to nonlocal collisions

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MAX-PLANCK-GESELLSCHAFT

Fluctuations in kinetic equations

How to describe sufficiently the fluctuations in dynamical systems ?
a) Stochasticity (Brownian motion) or b) Deterministic picture
In time evolution of one-particle distribution often additional stochastic term (Boltzmann - Langevin picture) [1–6]

$$\frac{df}{dt} = (1-f)W_{\rm in} - fW_{\rm out} + \delta I$$

from stochastic TDHF equation if one-particle reduced density traced out, assumed to be Markovian $\langle \delta I\rangle = 0$, $\langle \delta I(t)\delta I(t')\rangle = 2D\delta(t-t')$
variance $\sigma^2 = \langle f^2\rangle - \langle f\rangle^2$ with $1/\tau = W_{\rm out} + W_{\rm in}$

$$\frac{d\sigma^2}{dt} = -\frac{2}{\tau}\sigma^2 + 2D$$

educated guess [7]: $2D = (1-\langle f\rangle)W_{\rm in} + \langle f\rangle W_{\rm out}$ reproduce equilibrium variance $\sigma^2 = f_0(1-f_0)$
deviation $\delta\sigma^2 = \sigma^2 - \langle f\rangle(1-\langle f\rangle)$ obeys $\frac{d\delta\sigma^2}{dt} = -\frac{2}{\tau}\delta\sigma^2$.
Numerically density projection often used

$$\sigma_n^2(r,t) = s\int dp\langle f(p,r,t)\rangle(1-\langle f(p,r,t)\rangle)$$

which has been realized in each phase-space point.
• Same mean fluctuations from deterministic but more realistic nonlocal extension of Boltzmann collision integral [8–11].
Advantage:
Only one simple equation, systematical control in used approximations

Real-time Green functions

Two independent correlation functions $1 = r, t, s, \ldots$
$G^>(1,2) =< a(1)a^+(2) >$ and $G^<(1,2) =< a^+(2)a(1) >$

Martin Schwinger hierarchy for causal GF
$iG = \Theta(t_1-t_2)G^> \pm \Theta(t_2-t_1)G^<$

$$G_0^{-1}G(1,1') = \delta_{1,1'} + \int d3V(1,3)G_2(1,3,1',3^+) \equiv \delta_{1,1'} + \int_C d3\Sigma(1,3)G(3,1')$$

with $G_0^{-1}(11') = \left(i\frac{\partial}{\partial t_1} - \frac{(\frac{\hbar}{i}\nabla_{x_1})^2}{2m} - \Sigma^{HF}(11')\right)\delta(1-1')$

Weakening of initial correlations $\lim\limits_{t\to t_0}\Sigma G = 0$ leads to Keldysh contour
Consequence: Kadanoff and Baym equation (KB)

Gradient expansion of KB -equation

First order gradient expansion $t_1 - t_2 \to \omega$, $r_1 - r_2 \to k$

$$\left(\frac{\partial}{\partial t} + (\frac{p}{m} + \nabla_p\Sigma^{HF})\nabla_R - \nabla_R\Sigma^{HF}\nabla_p\right)\rho =$$
$$\int\frac{d\omega}{2\pi}(G^>_\omega\Sigma^<_\omega - G^<_\omega\Sigma^>_\omega) + \int\frac{d\omega d\omega'}{(2\pi)^2}\frac{P}{\omega'-\omega}(\{\Sigma^>_{\omega'}, G^<_\omega\} - \{\Sigma^<_{\omega'}, G^>_\omega\})$$
$$-\frac{\partial}{\partial t}\int\frac{d\omega' d\omega}{(2\pi)^2}\frac{P'}{\omega'-\omega}(G^>_\omega\Sigma^<_{\omega'} - G^<_\omega\Sigma^>_{\omega'}).$$

leads to quasiparticle distribution and iteration for Wigner function

$$\rho = \int\frac{d\omega}{2\pi}G^<_\omega \approx f - \int\frac{d\omega'}{2\pi}\frac{P'}{\omega'-\varepsilon}((1-f)\Sigma^<_{\omega'} - f\Sigma^>_{\omega'})$$

kinetic equation for quasiparticles

$$\frac{\partial}{\partial t}f + \nabla_k\varepsilon\nabla_R f - \nabla_R\varepsilon\nabla_k f = z\left((1-f)\Sigma^< - f\Sigma^>\right)$$

with wave function renormalization $\quad z = (1-\partial_\omega\Sigma)^{-1}$

$$\boxed{\rho = zf - \int\frac{d\omega}{2\pi}\frac{P'}{\omega-\varepsilon}\Sigma^<_\omega}$$

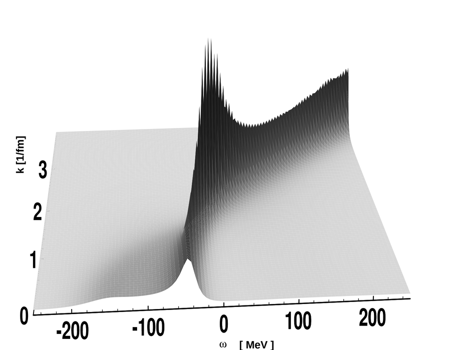
corresponds to extended quasiparticle picture

$$A = G^> - G^< = \frac{\Gamma_\omega}{[\omega - \frac{p^2}{2m} - \Sigma_\omega]^2 + \frac{1}{4}\Gamma^2_\omega} \approx 2\pi z\delta(\omega-\varepsilon) - \Gamma_\omega\frac{\partial}{\partial\omega}\frac{\mathcal{P}}{\omega-\varepsilon}$$

Equilibrium [12–17], Nonequilibrium [9, 18, 19]

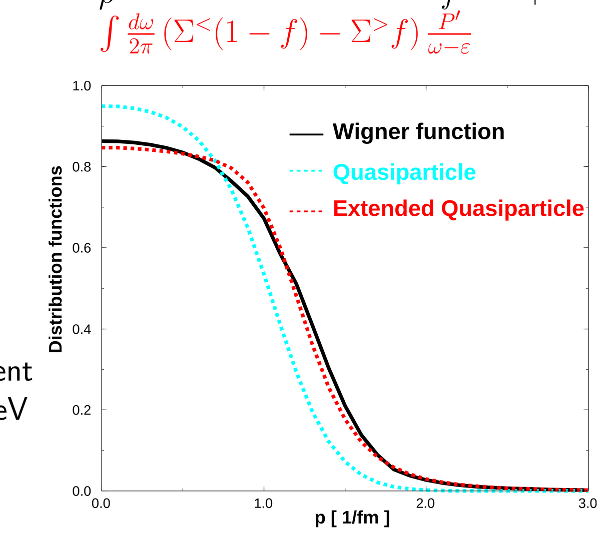
Message from Equilibrium

$$\rho(k) = \int\frac{d\omega}{2\pi}\frac{\Gamma(\omega,k)}{\left(\omega - \frac{k^2}{2m} - \Sigma(\omega,k)\right)^2 + \frac{1}{4}\Gamma(\omega,k)^2}f_{\rm FD}(\omega)$$



Spectral function for selfconsistent separable T-matrix at $T = 10$MeV

Extended Quasiparticle Picture
$\rho = f + \int\frac{d\omega}{2\pi}\left(\Sigma^<(1-f) - \Sigma^> f\right)\frac{P'}{\omega-\varepsilon}$



Non-local kinetic equation

Non-Markovian (memory) kinetic equation for reduced density ρ

$$\frac{\partial}{\partial t}\rho + \nabla_k\epsilon_{\rm HF}\nabla_r\rho - \nabla_r\epsilon_{\rm HF}\nabla_k\rho = \int\limits_0^{t-t_0}d\tau\left(\{G^<(t-\frac{\tau}{2},\tau), \Sigma^>(t-\frac{\tau}{2},-\tau)\} - \{G^>(t-\frac{\tau}{2},\tau), \Sigma^<(t-\frac{\tau}{2},-\tau)\}\right)$$

is transformed by extended quasiparticle picture into precursor of kinetic equation for quasiparticle distribution f

$$\frac{\partial}{\partial t}f + \nabla_k\epsilon\nabla_R f - \nabla_R\epsilon\nabla_k f = z\left((1-f)\Sigma^< - f\Sigma^>\right)$$

ladder summation: Boltzmann-Uehling-Uhlenbeck, each phase approximation: Lenard- Balescu equation, etc

But: non-local scattering events by $\Sigma[G] \to \Sigma[f]$
Memory or off-shell parts

- compensate the off-shell parts in Kadanoff Baym equation without other neglects
- in quasiparticle energy $\varepsilon_1 = \frac{k^2}{2m_a} + {\rm Re}\Sigma^R_{1,\varepsilon_1}$, off-shell part leads to the correct binding energy
- Wave function renormalization z
- A genuine time nonlocality Δ_t
- direct link between Wigner function (reduced density matrix) and quasi-particle distribution

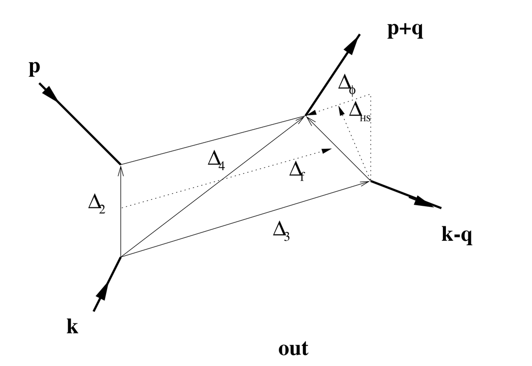
virial corrections from intrinsic gradients in the scattering integrals.

Consistent kinetic equation

$$\frac{\partial f_1}{\partial t} + \frac{\partial\varepsilon_1}{\partial k}\frac{\partial f_1}{\partial r} - \frac{\partial\varepsilon_1}{\partial r}\frac{\partial f_1}{\partial k} = \int\frac{dpdq}{(2\pi)^5}\mathcal{P}\,\delta\left(\varepsilon_1 + \varepsilon_2^- - \varepsilon_3^- - \varepsilon_4^- - 2\Delta_E\right)$$
$$\times\left[(1-f_1)(1-f_2^-)f_3^-f_4^- - f_1f_2^-(1-f_3^-)(1-f_4^-)\right]$$

where

$$\begin{aligned} f_1 &\equiv f(k,r,t)\\ f_2^- &\equiv f(p, r-\Delta_2, t)\\ f_3^- &\equiv f(k-q-\Delta_K, r-\Delta_3, t-\Delta_t)\\ f_4^- &\equiv f(p+q-\Delta_K, r-\Delta_4, t-\Delta_t)\end{aligned}$$



with T-matrix $\boxed{\mathbf{T}} = \,\vdots\, + \,\vdots\!\boxed{\mathbf{T}} = |\mathbf{T}|\,e^{i\phi}$

$$\mathcal{P} = \mathcal{Z}|\mathbf{T}|^2\left(\varepsilon_1+\varepsilon_2^- - \Delta_E, k - \frac{\Delta_K}{2}, p - \frac{\Delta_K}{2}, q, r - \frac{1}{4}(\Delta_2+\Delta_3+\Delta_4), t - \frac{\Delta_t}{2}\right)$$

$$\begin{aligned}\Delta_t &= \frac{\partial\phi}{\partial\Omega}\Big|_{\varepsilon_1+\varepsilon_2} & \Delta_2 &= \left(\frac{\partial\phi}{\partial p} - \frac{\partial\phi}{\partial q} - \frac{\partial\phi}{\partial k}\right)_{\varepsilon_1+\varepsilon_2}\\ \Delta_E &= -\frac{1}{2}\frac{\partial\phi}{\partial t}\Big|_{\varepsilon_1+\varepsilon_2} & \Delta_3 &= -\frac{\partial\phi}{\partial k}\Big|_{\varepsilon_1+\varepsilon_2}\\ \Delta_K &= \frac{1}{2}\frac{\partial\phi}{\partial r}\Big|_{\varepsilon_1+\varepsilon_2} & \Delta_4 &= -\left(\frac{\partial\phi}{\partial k} + \frac{\partial\phi}{\partial q}\right)_{\varepsilon_1+\varepsilon_2}\end{aligned}$$

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Summary of Correlated Observables

Quasiparticle parts (Landau theory – like)

$$\begin{aligned} n^{\rm qp} &= \sum_k f & \mathcal{Q}^{\rm qp} &= \sum_k k\,f & j^{\rm qp} &= \sum_k\frac{\partial\varepsilon}{\partial k}f\\ \mathcal{E}^{\rm qp} &= \sum_k(\frac{k^2}{2m} + \frac{1}{2}\Sigma_{mf})f_k & \mathcal{J}^{\rm qp}_{ij} &= \sum_k\left(k_j\frac{\partial\varepsilon}{\partial k_i} + \delta_{ij}\varepsilon\right)f - \delta_{ij}\mathcal{E}^{\rm qp}\end{aligned}$$

Two-particle correlated parts with probability to form a molecule per time $d\mathcal{P} = \delta_{1234}|t_{\rm sc}|^2 f_1f_2(1-f_3-f_4)$

$$\begin{aligned} n^{\rm mol} &= \int d\mathcal{P}\,\Delta_t & j^{\rm mol} &= \int d\mathcal{P}\,\Delta_3\\ \mathcal{Q}^{\rm mol} &= \int d\mathcal{P}\frac{k+p}{2}\Delta_t & \mathcal{E}^{\rm mol} &= \int d\mathcal{P}\frac{\epsilon_k+\epsilon_p}{2}\Delta_t\end{aligned}$$
$$\mathcal{J}^{\rm mol}_{ij} = \frac{1}{2}\int d\mathcal{P}\left\{k_j\Delta_{3i} + p_j(\Delta_{4i} - \Delta_{2i}) + q_j(\Delta_{4i} - \Delta_{3i})\right\}$$

Conservation laws

$$\begin{aligned}\frac{\partial(n^{\rm qp} + n^{\rm mol})}{\partial t} + \frac{\partial(j^{\rm qp} + j^{\rm mol})}{\partial r} &= 0\\ \frac{\partial(\mathcal{Q}^{\rm qp}_i + \mathcal{Q}^{\rm mol}_i)}{\partial t} + \sum_i\frac{\partial(\mathcal{J}^{\rm qp}_{ij} + \mathcal{J}^{\rm mol}_{ij})}{\partial r_i} &= 0\\ \frac{\partial\mathcal{E}}{\partial t} = \frac{\partial(\mathcal{E}^{\rm qp} + \mathcal{E}^{\rm mol})}{\partial t} &= 0\end{aligned}$$

Internal energy- $\mathcal{I}_{\rm gain} = \int d\mathcal{P}\Delta_E$ and momentum–gain $\mathcal{F}^{\rm gain} = \int d\mathcal{P}\Delta_K$

Additional mean-field channel

Zero momentum transfer channel $q = 0$ leads to an additional part absent in usual local Boltzmann kinetic equation

$$\lim_{q=0}\left[(1-f_1)(1-f_2^-)f_3^-f_4^- - f_1f_2^\pm(1-f_3^\pm)(1-f_4^\pm)\right] = f_2^-(1-f_2^-)\left[f_1^- - f_1\right]$$

we obtain now $\frac{\partial f_1}{\partial t} + \frac{\partial\varepsilon_1}{\partial k}\frac{\partial f_1}{\partial r} - \frac{\partial\varepsilon_1}{\partial r}\frac{\partial f_1}{\partial k} = \frac{\langle f_1^- - f_1\rangle}{\tilde\tau} + \mathcal{I}^{\rm nonlocal}_{\rm coll}(q\neq 0)$ used thermal averaged delays, $\langle\ldots\rangle$ for legibility
• additional term represents mean-field fluctuations

$$\langle f_1 - f_1^-\rangle = \langle\Delta_t\frac{\partial f}{\partial t} + \Delta_3\frac{\partial f}{\partial r} + \Delta_K\frac{\partial f}{\partial k}\rangle \approx \tilde\Delta_3\frac{\partial f}{\partial r} + \tilde\Delta_K\frac{\partial f}{\partial k}$$

which on-shell $\tilde\Delta_3 = \langle\Delta_3 - \Delta_t\frac{\partial\varepsilon_k}{\partial k}\rangle = -\langle\frac{\partial\phi^{\rm on}}{\partial k}\rangle$ and $\tilde\Delta_K = \langle\Delta_K + \Delta_t\frac{\partial\varepsilon_k}{\partial r}\rangle = \langle\frac{\partial\phi^{\rm on}}{\partial r}\rangle$ arrive finally [20]

$$\frac{\partial f_1}{\partial t} + \left(\frac{\partial\varepsilon_1}{\partial k} + \frac{\tilde\Delta_3}{\tilde\tau}\right)\frac{\partial f_1}{\partial r} - \left(\frac{\partial\varepsilon_1}{\partial r} - \frac{\tilde\Delta_K}{\tilde\tau}\right)\frac{\partial f_1}{\partial k} = \mathcal{I}^{\rm nonlocal}_{\rm coll}(q\neq 0)$$

• An explicit fluctuating term $1/\tilde\tau \sim \sigma_n^2(r,t)$ emerges to the mean field

Bifurcation in time evolution

For homogeneous systems and relaxation time approximation: additional term in the kinetic equation [21]

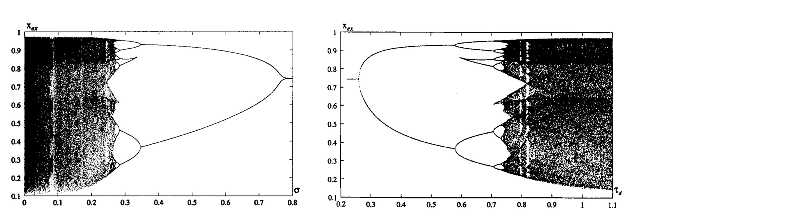
$$\frac{df(k,t)}{dt} = -\frac{f(k,t) - F_0}{\tau} + \frac{f(k,t-\Delta_t)[1 - f(k,t-\Delta_t)]}{\tilde\tau}$$

with thermal averaging $< \ldots >$

$$\begin{aligned}\frac{1}{\tau} &= \langle s\int\frac{dpdq}{(2\pi)^5}|\mathcal{T}^r(k,p,q)|^2\delta(\varepsilon_k+\varepsilon_p-\varepsilon_{k+q}-\varepsilon_{p-q})f_p(1-f_{k-q})(1-f_{p+q})\rangle\\ \frac{1}{\tilde\tau} &= \langle s\int\frac{dpdq}{(2\pi)^5}|\mathcal{T}^r(k,p,q)|^2\delta((k-p)\cdot\frac{q}{m})f_p(1-f_p)\rangle\\ \Delta_t &= -\langle\frac{\partial}{\partial\omega}{\rm Im}\ln\mathcal{T}^r(k,p,q,\omega)|_{\omega=\varepsilon_k+\varepsilon_p}\rangle\end{aligned}$$

Rename $\alpha = \frac{\tau}{\tilde\tau}\quad\sigma = \tau\quad\tau_d = \Delta_t$ to obtain [22]

$$\sigma\frac{df(t)}{dt} + f(t) = \alpha f(t-\tau_d)[1 - f(t-\tau_d)]$$



Feigenbaum diagram $\alpha = 3.9, \tau_d = 1$ (left) and $\alpha = 3.9$, $\sigma = 0.2$ (right)
Bifurcation sets in for $|\alpha - 2| \gtrless \sqrt{1 + (\sigma\Omega)^2}$ for $\tau_d \gtrless 0$ and oscillation appears with a frequency

$$\tau_d\Omega + \arctan(\sigma\Omega) = \pi$$

Summary

1. Non-local collisions in quantum kinetic equation
   - Unifies Landau-quasiparticle transport and Enskog equations for dense gases
   - Thermodynamically consistent equation of state (energy, density, pressure) including quantum 2. virial coefficient
   - Quantum correlation recast into quasi-classical picture
   - Particle-hole vs space-time symmetry completed
   - Modify existing Boltzmann codes by nonlocal and non-instantaneous shifts tabulated from two-particle scattering data
   - Delay differential equation interpolate between finite time stepping of the logistic map and continuous time derivatives [21], Novel observation: distribution function itself shows temporal oscillations around the equilibrium value, bifurcation, signal of onsetting phase transition
2. Memory effects result in
   - Off-shell tails of Wigner function (exactly compensated)
   - Renormalization of scattering rates
   - Collision delay is all what is left from memory
   - Related non-local corrections to the scattering integral
3. We have successfully applied it to: Heavy Ion collisions, deep neutral impurities, Bernoulli potential at superconducting surfaces