Nonlocal Quantum Kinetic Theory

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Real-time Green functions

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

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

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

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

$$\int_{\mathcal C} d\bar 1\Sigma(1,\bar 1)G(\bar 1,1') = \int_{-\infty}^{+\infty} d\bar 1\left\{\Sigma(1,\bar 1)G(\bar 1,1') - \Sigma^<(1,\bar 1)G^>(\bar 1,1')\right\}$$

Consequence: Kadanoff and Baym equation (KB)

$$-i\left(G_0^{-1}G^< - G^<G_0^{-1}\right)(t_1,t_2) = \int_{t_0}^{t_1}\Sigma^>G^< + \int_{t_0}^{t_2}G^<\Sigma^> - \int_{t_0}^{t_1}G^>\Sigma^< - \int_{t_0}^{t_2}\Sigma^<G^> + \int_{t_1}^{t_2}[\Sigma^<,G^<]$$

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

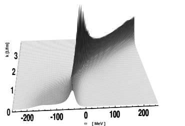
$$A = G^> - G^< = \frac{\Gamma_\omega}{[\omega - \frac{p^2}{2m} - \Sigma_\omega]^2 + \frac14\Gamma^2_\omega} \approx 2\pi z\delta(\omega-\varepsilon) - \Gamma_\omega\frac{\partial}{\partial\omega}\frac{\mathcal P}{\omega-\varepsilon}$$

Equilibrium:
Craig '66, Bezzerides DeBois '68, Zimmermann, Stolz'79,Kremp '84, Röpke, Schmidt '87, Köhler, Malfliet '93
Nonequilibrium:
Lipavský, Špička 1995, Morawetz '00

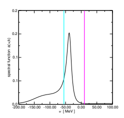
Message from Equilibrium

$$\rho(k) = \int\frac{d\omega}{2\pi}\frac{\Gamma(\omega,k)}{\left(\omega - \frac{k^2}{2m} - \Sigma(\omega,k)\right)^2 + \frac14\Gamma(\omega,k)^2}f_{\rm FD}(\omega)$$

example from nuclear matter

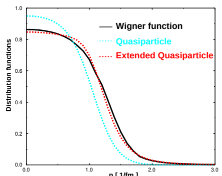


Spectral function for selfconsistent separable T-matrix at $T = 10$MeV



Full spectral function $k = 0.7$ fm^{-1}, free particle, Hartree Fock .

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

$$\frac{\partial}{\partial t}\rho + \nabla_k\epsilon_{\rm HF}\nabla_r\rho - \nabla_r\epsilon_{\rm HF}\nabla_k\rho = \int_0^{t-t_0}d\tau\left(\{G^<(t-\frac{\tau}{2},\tau),\Sigma^>(t-\frac{\tau}{2},-\tau)\} - \{G^>(t-\frac{\tau}{2},\tau),\Sigma^<(t-\frac{\tau}{2},-\tau)\}\right)$$

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, random 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

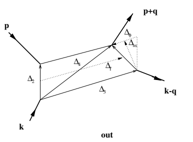
virial corrections from intrinsic gradients in the scattering integrals.

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

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



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

$$\mathcal P = z_1z_2z_3z_4|\mathbf T|^2\left(\varepsilon_1 + \varepsilon_2^- - \Delta_E, k - \frac{\Delta_K}{2}, p - \frac{\Delta_K}{2}, q, r - \frac14(\Delta_2 + \Delta_3 + \Delta_4), t - \frac{\Delta_t}{2}\right)$$

$$\Delta_t = \frac{\partial\phi}{\partial\Omega}\Big|_{\varepsilon_1+\varepsilon_2} \qquad \Delta_2 = \left(\frac{\partial\phi}{\partial p} - \frac{\partial\phi}{\partial q} - \frac{\partial\phi}{\partial k}\right)_{\varepsilon_1+\varepsilon_2}$$
$$\Delta_E = -\frac12\frac{\partial\phi}{\partial t}\Big|_{\varepsilon_1+\varepsilon_2} \qquad \Delta_3 = -\frac{\partial\phi}{\partial k}\Big|_{\varepsilon_1+\varepsilon_2}$$
$$\Delta_K = \frac12\frac{\partial\phi}{\partial r}\Big|_{\varepsilon_1+\varepsilon_2} \qquad \Delta_4 = -\left(\frac{\partial\phi}{\partial k} + \frac{\partial\phi}{\partial q}\right)_{\varepsilon_1+\varepsilon_2}$$

P. Lipavský, K. M., and V. Špička: *Kinetic equation for strongly interacting dense Fermi systems*, Annales de physique, 26,1 (2001) ISBN 2-86883-541-4

Nonequilibrium thermodynamics from balance

Quasiparticle parts (Landau theory – like)

$$n^{\rm qp} = \sum_k f \qquad \mathcal Q^{\rm qp} = \sum_k k\,f \qquad j^{\rm qp} = \sum_k\frac{\partial\varepsilon}{\partial k}f$$
$$\mathcal E^{\rm qp} = \sum_k(\frac{k^2}{2m} + \frac12\Sigma_{mf})f_k \qquad \mathcal J^{\rm qp}_{ij} = \sum_k\left(k_j\frac{\partial\varepsilon}{\partial k_i} + \delta_{ij}\varepsilon\right)f - \delta_{ij}\mathcal E^{\rm qp}$$

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

$$n^{\rm mol} = \int d\mathcal P\,\Delta_t \qquad j^{\rm mol} = \int d\mathcal P\,\Delta_3$$
$$\mathcal Q^{\rm mol} = \int d\mathcal P\,\frac{k+p}{2}\Delta_t \qquad \mathcal E^{\rm mol} = \int d\mathcal P\,\frac{\epsilon_k+\epsilon_p}{2}\Delta_t$$
$$\mathcal J^{\rm mol}_{ij} = \frac12\int d\mathcal P\left\{k_j\Delta_{3i} + p_j(\Delta_{4i} - \Delta_{2i}) + q_j(\Delta_{4i} - \Delta_{3i})\right\}$$

Conservation laws

$$\frac{\partial(n^{\rm qp} + n^{\rm mol})}{\partial t} + \frac{\partial(j^{\rm qp} + j^{\rm mol})}{\partial r} = 0$$
$$\frac{\partial(\mathcal Q^{\rm qp}_j + \mathcal Q^{\rm mol}_j)}{\partial t} + \sum_i\frac{\partial(\mathcal J^{\rm qp}_{ij} + \mathcal J^{\rm mol}_{ij})}{\partial r_i} = 0$$
$$\frac{\partial(\mathcal E^{\rm qp} + \mathcal E^{\rm mol})}{\partial t} + \frac{\partial(j^{\rm qp}_E + j^{\rm mol}_E)}{\partial r} = 0$$

- Binary quantum-correlation part to observables from extended quasiparticle picture coincides with balance from nonlocal kinetic equation $\to$ consistency

Energy conversion: latent heat

There appear an internal energy- $\mathcal I_{\rm gain} = \int d\mathcal P\Delta_E$ and momentum–gain $\mathcal F^{\rm gain} = \int d\mathcal P\Delta_K$

From nonlocal kinetic equation

$$\int\frac{dk}{(2\pi)^3}\varepsilon_k\frac{\partial f_k}{\partial t} = -\frac{d}{dt}\int d\mathcal P\frac{\varepsilon_k + \varepsilon_p}{2}\Delta_t + \int d\mathcal P\Delta_E$$

energy gain combines together with drift term into time derivative

$$\sum_a\int\frac{dk}{(2\pi)^3}\varepsilon\frac{\partial f}{\partial t} - \mathcal I^E_{\rm gain} = \frac{\partial\mathcal E^{\rm qp}}{\partial t}.$$

of the quasiparticle energy functional

$$\mathcal E^{\rm qp} = \sum_a\int\frac{dk}{(2\pi)^3}f_a(k)\frac{k^2}{2m} + \frac12\sum_{ab}\int\frac{dkdp}{(2\pi)^6}f_a(k)f_b(p)\mathcal T_{\rm ex}(\varepsilon_1 + \varepsilon_2, k, p, 0)$$

- By energy gain $\Delta_E = \frac{\partial\Phi}{\partial t}$ transformation of kinetic energy into correlation energy, Similar to breathing hard-sphere by Pauli-blocking

Entropy balance

$$\frac{\partial(\mathcal S^{\rm qp} + \mathcal S^{\rm mol})}{\partial t} + \frac{\partial(\mathbf j^{\rm qp}_S + \mathbf j^{\rm mol}_S)}{\partial\mathbf r} = \mathcal I^S_{\rm gain}$$

quasiparticle part $\mathcal S^{\rm qp} = -k_B\int\frac{dk}{(2\pi)^3}[f_1\ln f_1 + (1\mp f_1)\ln(1\mp f_1)]$
molecular part $\mathcal S^{\rm mol} = -\frac{k_B}{2}\int d\mathcal P f_1f_2(1\mp f_3\mp f_4)\ln\frac{f_3f_4}{(1\mp f_3)(1\mp f_4)}$
entropy gain

$$\mathcal I^S_{\rm gain} = -\frac{k_B}{2}\sum_{ab}\int d\mathcal P f_1f_2(1\mp f_3)(1\mp f_4)\ln\frac{f_3f_4(1\mp f_1)(1\mp f_2)}{(1\mp f_3)(1\mp f_4)f_1f_2} \geq 0$$

- H-theorem holds also for nonlocal kinetic theory

Relation to Landau theory

Landau theory works only if collisions $\bar I$ treated instant and local
From kinetic equation $\frac{\partial\bar f_k}{\partial t} = \bar I_k$ follows:

number of particles

$$\frac{dn}{dt} = \int\frac{dk}{(2\pi)^3}\frac{\partial\bar f_k}{\partial t} = \int\frac{dk}{(2\pi)^3}\bar I_k = 0$$

energy balance

$$\frac{d\mathcal E}{dt} = \int\frac{dk}{(2\pi)^3}\frac{\delta\mathcal E}{\delta\bar f_k}\frac{\partial\bar f_k}{\partial t} = \int\frac{dk}{(2\pi)^3}\bar\varepsilon_k\bar I_k = 0$$

Nonlocal kinetic theory

$$\frac{dn}{dt} = \frac{d}{dt}\int\frac{dk}{(2\pi)^3}f_k + \cancel{\frac{d}{dt}\int d\mathcal P\Delta_t}$$
$$\frac{d\mathcal E}{dt} = \int\frac{dk}{(2\pi)^3}\varepsilon_k\frac{\partial f_k}{\partial t} + \cancel{\frac{d}{dt}\int d\mathcal P\frac{\varepsilon_k+\varepsilon_p}{2}\Delta_t} - \int d\mathcal P\Delta_E$$

Instant approximation, last term can be rewritten $\Delta_E = -\frac12\frac{\partial\phi}{\partial t}$

$$-\int d\mathcal P\Delta_E = \frac12\int d\mathcal P\frac{\partial\phi}{\partial t} = \int\frac{dk}{(2\pi)^3}\int d\mathcal P\frac{\delta\phi}{\delta\bar f_k}\frac{\partial\bar f_k}{\partial t} \equiv \int\frac{dk}{(2\pi)^3}\epsilon^\Delta_k\frac{\partial\bar f_k}{\partial t}$$

with rearrangement energy
follows variational expression of Landau theory $\bar\varepsilon_k = \varepsilon_k + \epsilon^\Delta_k$
Landau theory mimes for energy gain, but no correlated density !

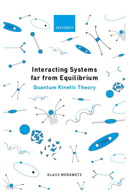
Summary

1. Non-local collisions in quantum kinetic equation
   - Unifies Landau - quasiparticle and Enskog - like equations
   - 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
   - Consistent theory unifying Landau theory and dense gases
   - Explicit calculation of Wigner function not necessary, correlated observables directly from nonlocal kinetic equation
   - No additional computational expenses
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
3. Successfully applied to: Heavy Ion collisions, deep neutral impurities, Bernoulli potential at superconducting surfaces, ...

Literature:

http://www.pks.mpg.de/~morawetz

Book 2017



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