Nonlocal Kinetic Theory

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MAX-PLANCK-GESELLSCHAFT

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 $G_0^{-1}(11') = \left(i\frac{\partial}{\partial t_1} - \frac{(\frac{1}{i}\nabla_{r_1})^2}{2m} - \Sigma^{HF}(11')\right)\delta(1-1')$

Weakening of initial correlations $\lim_{t\to t_0} \Sigma G = 0$ 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 $z = (1 - \partial_\omega\Sigma)^{-1}$

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

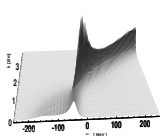
corresponds to extended quasiparticle picture

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

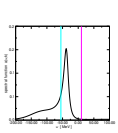
Equilibrium:
Craig '66, Bezzerides DeBois '68, Zimmermann, Stolz'79,Kremp '84, Röpke, Schmidt '87, Köhler, Malfliet '93
Nonequilibrium:
Lipavský, Špička 1995, Morawetz '00

Message from Equilibrium

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

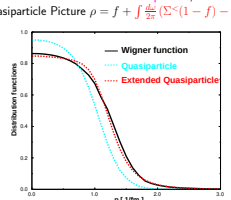


Spectral function for selfconsistent separable T-matrix at $T = 10$MeV



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

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



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 $\varepsilon_1 = \frac{k^2}{2m_a} + \mathrm{Re}\Sigma^R_{1,\varepsilon_1}$, 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 quasiparticle distribution

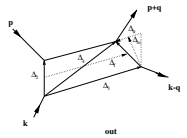
virial corrections from intrinsic gradients in the scattering integrals.

Consistent kinetic equation

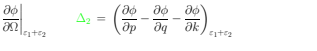
$$\frac{\partial f_1}{\partial t} + \frac{\partial\varepsilon_1}{\partial k}\frac{\partial f_1}{\partial r} - \frac{\partial\varepsilon_1}{\partial r}\frac{\partial f_1}{\partial k} = \int\frac{dpdq}{(2\pi)^6}\mathcal{P}\,\delta\left(\varepsilon_1 + \varepsilon_2^- - \varepsilon_3^- - \varepsilon_4^- - 2\Delta_E\right) \times\left[\left(1-f_1\right)\left(1-f_2^-\right)f_3^-f_4^- - f_1f_2^-\left(1-f_3^-\right)\left(1-f_4^-\right)\right]$$

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



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

$$\Delta_t = \frac{\partial\phi}{\partial\Omega}\Big|_{\varepsilon_1+\varepsilon_2} \qquad \Delta_2 = \left(\frac{\partial\phi}{\partial p} - \frac{\partial\phi}{\partial q} - \frac{\partial\phi}{\partial k}\right)_{\varepsilon_1+\varepsilon_2}$$

$$\Delta_E = -\frac{1}{2}\frac{\partial\phi}{\partial t}\Big|_{\varepsilon_1+\varepsilon_2} \qquad \Delta_3 = -\frac{\partial\phi}{\partial k}\Big|_{\varepsilon_1+\varepsilon_2}$$

$$\Delta_K = \frac{1}{2}\frac{\partial\phi}{\partial r}\Big|_{\varepsilon_1+\varepsilon_2} \qquad \Delta_4 = -\left(\frac{\partial\phi}{\partial k} + \frac{\partial\phi}{\partial q}\right)_{\varepsilon_1+\varepsilon_2}$$

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

Summary of Correlated Observables

Quasiparticle parts (Landau theory – like)

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

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

$$n^{\rm mol} = \int d\mathcal{P}\,\Delta_t \qquad j^{\rm mol} = \int d\mathcal{P}\,\Delta_3$$
$$\mathcal{Q}^{\rm mol} = \int d\mathcal{P}\,\frac{k_1+p}{2}\Delta_t \qquad \mathcal{E}^{\rm mol} = \int d\mathcal{P}\,\frac{\varepsilon_k+\varepsilon_p}{2}\Delta_t$$
$$\mathcal{J}_{ij}^{\rm mol} = \frac{1}{2}\int d\mathcal{P}\left\{k_j\Delta_{3i} + p_j(\Delta_{4i} - \Delta_{2i}) + q_j(\Delta_{4i} - \Delta_{3i})\right\}$$

Conservation laws

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

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

Two concepts of quasiparticles

Landau theory

number of particles = number of quasiparticles

$$n = \int\frac{dk}{(2\pi)^3}\tilde{f}_k$$

Quasiparticle energy

$$\tilde{\epsilon}_k = \frac{\delta\mathcal{E}}{\delta\tilde{f}_k}$$

Beth-Uhlenbeck equation of state '37

number of particles = number of free + bound particles

$$n = n_f + 2n_i^3B(n,T)$$

$$\sim\sum_{\alpha,E}c_\alpha e^{-E/T}\left[\delta(E-E_\alpha) + \frac{1}{\pi}\frac{d}{dE}\phi_\alpha(E)\right]$$

with two-particle scattering phase shift ϕ

Spectral concept

Quasiparticle energy as pole part $\varepsilon = \frac{k^2}{2m} + \Sigma(k,\varepsilon)$

$$A = \frac{\Gamma}{(\omega - \frac{k^2}{2m} - \Sigma)^2 + \frac{1}{4}\Gamma^2} \approx \left(1 + \frac{\partial\Sigma}{\partial\omega}\right)2\pi\delta(\omega-\varepsilon) + \frac{\varepsilon'}{\omega-\varepsilon}\Gamma$$

In extended quasiparticle picture

$$n = \int\frac{d\omega}{2\pi}A\,f_{\rm FD} = \int\frac{dk}{(2\pi)^3}f_k + \int d\mathcal{P}\Delta_t$$

Total density = quasiparticle density + correlated density

- Coincides with balance from nonlocal kinetic equation → consistency
- Explicit calculation of Wigner function not necessary, correlated observables directly from quasiparticle kinetic equation

Relation to Landau theory

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

number of particles

$$\frac{dn}{dt} = \int\frac{dk}{(2\pi)^3}\frac{\partial\tilde{f}_k}{\partial t} = \int\frac{dk}{(2\pi)^3}\tilde{I}_k = 0$$

energy balance

$$\frac{d\mathcal{E}}{dt} = \int\frac{dk}{(2\pi)^3}\frac{\delta\mathcal{E}}{\delta\tilde{f}_k}\frac{\partial\tilde{f}_k}{\partial t} = \int\frac{dk}{(2\pi)^3}\tilde{\varepsilon}_k\tilde{I}_k = 0$$

Nonlocal kinetic theory

$$\frac{dn}{dt} = \frac{d}{dt}\int\frac{dk}{(2\pi)^3}f_k + \frac{d}{dt}\int d\mathcal{P}\Delta_t$$

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

Instant approximation, last term can be rewritten $\Delta_E = -\frac{1}{2}\frac{\partial\phi}{\partial t}$

$$-\int d\mathcal{P}\Delta_E = \frac{1}{2}\int d\mathcal{P}\frac{\partial\phi}{\partial t} = \int\frac{dk}{(2\pi)^3}\int d\mathcal{P}\frac{\delta\phi}{\delta\tilde{f}_k}\frac{\partial\tilde{f}_k}{\partial t} \equiv \int\frac{dk}{(2\pi)^3}\tilde{\varepsilon}_k\frac{\partial\tilde{f}_k}{\partial t}$$

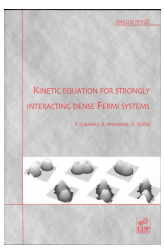
with rearrangement energy
follows variational expression of Landau theory

$$\tilde{\varepsilon}_k = \varepsilon_k + \epsilon_k^{\Delta}$$

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
   - No additional computational expenses -modify existing Boltzmann codes by nonlocal and non-instantaneous shifts -shifts tabulated from two-particle scattering data
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



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Literature:
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