Formation of (initial) correlations

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MAX-PLANCK-GESELLSCHAFT

Introduction

1. Formation of correlations and screening at short times
2. Initial correlations
3. Exact equivalence between N particle classical and N-1 particle quantum systems
4. Derive effective quantum potentials (Kelbg and higher order)
5. Conjecture: Dense classical systems can be described by Quantum Born calculations replacing quantum parameter by classical ones
6. Test: Simulation of one component plasma

Non-Markovian kinetic equation

Time diagonal part of Kadanoff/Baym equation Levinson equation

$$\frac{\partial}{\partial t}f_a(t) = \frac{2}{\hbar^2}\sum_b\int\frac{dpdq}{(2\pi\hbar)^6}V_D^2(q)\int_0^t d\bar t\,\exp\left\{-\frac{t-\bar t}{\tau}\right\}\cos\left\{\frac{1}{\hbar}(t-\bar t)\Delta_E\right\}\times\left\{\bar f'_a\bar f'_b(1-\bar f_a)(1-\bar f_b)-\bar f_a\bar f_b(1-\bar f'_a)(1-\bar f'_b)\right\}_{\bar t},$$

where $\Delta_E=\frac{k^2}{2m_a}+\frac{p^2}{2m_b}-\frac{(k-q)^2}{2m_a}-\frac{(p+q)^2}{2m_b}$

- particle-number, momentum conservation $\frac{\partial}{\partial t}n=0,\ \frac{\partial}{\partial t}\langle p_1\rangle=0.$
- Energy conservation if no damping [1]: $\frac{\partial}{\partial t}(\langle\frac{p_1^2}{2m}\rangle+\langle V_{12}\rangle)\equiv 0$
- Attention: Double count of correlations in Levinsonequation [7]

Solution at transient time regime

Analytical solution of Levinson's equation at short-times $t\ll\tau$

- neglect of time evolution of distributions, $\bar f_a(t)=f_a(0)$
- life-time factor, $\exp\left\{-\frac{t-\bar t}{\tau}\right\}=1$

deviation from initial value, $f_a(t)=f_a(0)+\delta f_a(t)$, reads

$$\delta f_a(t) = 2\sum_b\int\frac{dpdq}{(2\pi\hbar)^6}V_D^2(q)\frac{1-\cos\left\{\frac{1}{\hbar}t\Delta_E\right\}}{\Delta_E^2}\times\left\{f'_af'_b(1-f_a)(1-f_b)-f_af_b(1-f'_a)(1-f'_b)\right\}$$

two-particle and the single-particle concept of the transient behavior meet in kinetic equation

- right hand side: two particles correlate their motion to avoid the strong interaction regions
- Since process is very fast, the on-shell contribution to δf_a, has pure off-shell character
- off-shell character of mutual two-particle correlation is thus reflected in the single particle Wigner's distribution

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Paper available: http://www.mpipks-dresden.mpg.de/~morawetz

Books:

• P. Lipavský, K. Morawetz, and V. Špička, *Kinetic equation for strongly interacting dense Fermi systems* (Annales de Physique, Paris, 2001), No. 26, 1, ISBN:2-86883-541-4.

• K. Morawetz (ed.), *Nonequilibrium Physics at Short Time Scales* (Springer 2004), ISBN 3-540-20031-2

One component plasma

Time dependent formation analytically from kinetic theory [2–4]

static Debye with $z=\omega_p\sqrt{t^2-it\frac{\hbar}{T}}$.

$$\frac{\partial}{\partial t}E_{\rm corr}(t) = -\frac{e^2n\kappa T}{2}\frac{1}{\hbar}{\rm Im}\left[(1+2z^2)e^{z^2}(1-{\rm erf}(z))-\frac{2z}{\sqrt\pi}\right]$$

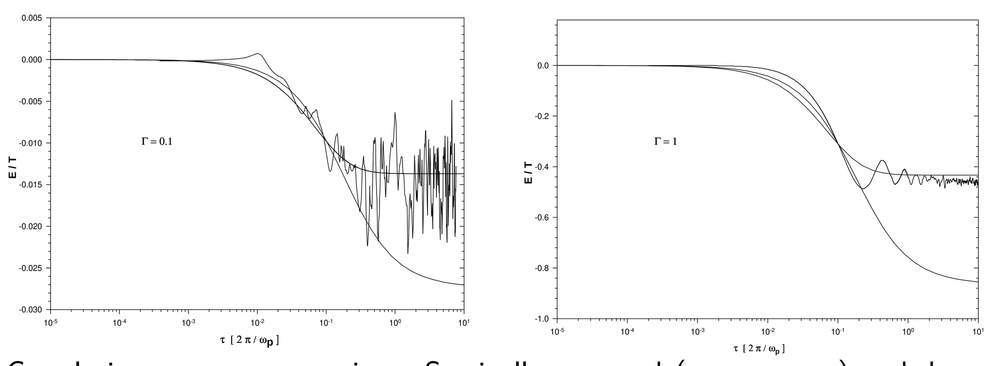
dynamical screening with $z_1=\omega_p\sqrt{2t^2-it\frac{\hbar}{T}}$

$$\frac{\partial}{\partial t}\frac{E^{\rm dynam}_{\rm corr}(t)}{n} = -\frac{e^2\kappa T}{\hbar}{\rm Im}\left[e^{z_1^2}(1-{\rm erf}(z_1))\right]$$

classical limit

$$E^{\rm static}_{\rm corr}(t) = -\frac{1}{4}\kappa e^2n\left[1+\frac{2\omega_pt}{\sqrt\pi}-(1+2(\omega_pt)^2)e^{(\omega_pt)^2}(1-{\rm erf}(\omega_pt))\right]$$

$$E^{\rm dynam}_{\rm corr}(t) = -\frac{1}{2}e^2n\kappa\left\{1-\exp\left(\frac{\omega_p^2}{2}t^2\right)\left[1-{\rm erf}\left(\frac{\omega_p}{\sqrt2}t\right)\right]\right\}.$$



Correlation energy versus time. Statically screened (upper curve) and dynamically screened (lower curve) are compared with moleculardynamical simulations [5,6].

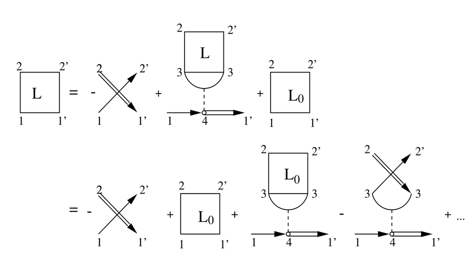
Initial correlations

Density correlation function $<\delta n(11^+)\delta n(22^+)>=L^<(121^+2^+)$

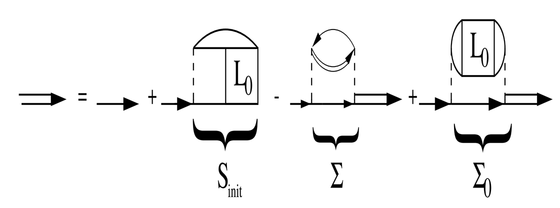
$$L(121'2')=(g_2(121'2')-g_1(11')g_1(22'))$$

Neglecting G_3
with $(G^R_{HF})^{-1}L_0=0$

Born approximation
Dyson equation reads



$$G_H^{-1}(1,3)G(3,2)=\delta(1-2)+\int d3V(1,3)L(1,3,2,3^+)$$



New type of self energy induced by initial correlations
Kinetic equation with GKB ansatz

$$\frac{\partial}{\partial t}\rho_k(t)=\frac{2}{\hbar^2}{\rm Re}\int_{t_0}^t dt_1\int\frac{dq}{(2\pi\hbar)^3}V^2(q)$$
$$\times\left\{\int\frac{dp}{(2\pi\hbar)^3}G^R(t,t_1,k-q)G^A(t_1,t,k)G^R(t,t_1,p+q)G^A(t_1,t,p)\right.$$
$$\times[\rho_{k-q}\rho_{p+q}(1-\rho_p)(1-\rho_k)-(1-\rho_{k-q})(1-\rho_{p+q})\rho_p\rho_k]_{t_1}$$
$$\left.+\mathcal{L}_0(q,t,t_1)G^R(t,t_1,k-q)G^A(t_1,t,k)[\rho_{k-q}(1-\rho_k)-(1-\rho_{k-q})\rho_k]_{t_1}\right\}$$
$$+\frac{2}{\hbar}{\rm Im}\int\frac{dqdp}{(2\pi\hbar)^6}V(q)G^R(t,t_0,k-q)G^A(t,t_0,k)G^R(t,t_0,p+q)G^A(t,t_0,p)$$
$$\times\langle\frac{p-k}{2}+q|L_{00}(p+k,t_0)|\frac{p-k}{2}\rangle,$$

Kinetic equation with initial correlations

L_{00} in first Born approximation

$$\left\langle\frac{k-p}{2}|L_{00}(k+p)|\frac{k-p}{2}-q\right\rangle=-\frac{\mathcal P}{\Delta\epsilon}V_0(q)\times\{\rho_{k-q}\rho_{p+q}(1-\rho_p-\rho_k)-\rho_k\rho_p(1-\rho_{p+q}-\rho_{k-q})\}_{t_0}$$

Result

$$\begin{aligned}\frac{\partial}{\partial t}\rho_k(t) &= \frac{2}{\hbar^2}\int_{t_0}^t dt_1\int\frac{dqdp}{(2\pi\hbar)^6}V^2(q)\\ &\times\cos\left[\left(\frac{k^2}{2m}+\frac{p^2}{2m}-\frac{(k-q)^2}{2m}-\frac{(p+q)^2}{2m}\right)\frac{(t-t_1)}{\hbar}\right]\\ &\times\{\rho_{k-q}\rho_{p+q}(1-\rho_p-\rho_k)-\rho_k\rho_p(1-\rho_{p+q}-\rho_{k-q})\}_{t_1}\\ &-\frac{2}{\hbar^2}\int_{t_0}^t dt_1\int\frac{dqdp}{(2\pi\hbar)^6}V(q)V_0(q)\\ &\times\cos\left[\left(\frac{k^2}{2m}+\frac{p^2}{2m}-\frac{(k-q)^2}{2m}-\frac{(p+q)^2}{2m}\right)\frac{(t-t_1)}{\hbar}\right]\\ &\times\{\rho_{k-q}\rho_{p+q}(1-\rho_p-\rho_k)-\rho_k\rho_p(1-\rho_{p+q}-\rho_{k-q})\}_{t_0}\end{aligned}$$

no evolution if ρ_0 already equilibrium

Analytic results

- Yukawa potential $V(q)=\frac{4\pi e^2\hbar^2}{q^2+\hbar^2\kappa_D^2}$ with $x=\kappa_D/\kappa$, $x\to 0$Coulomb
- Initial correlation $V_0(q)=\frac{4\pi e^2\hbar^2}{q^2+\hbar^2\kappa_0^2}$ with $x_0=\kappa_0/\kappa$
- Maxwellian plasma

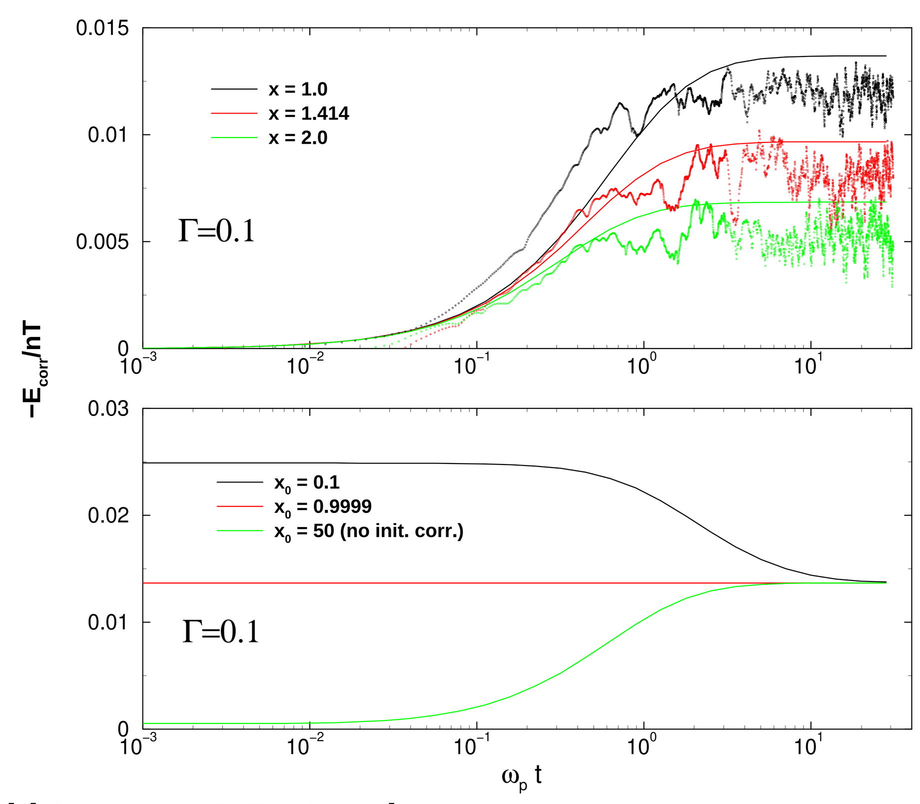
Time dependent kinetic energy

$$\frac{\partial}{\partial t}E_{\rm kin}(t)=\mathcal{E}[V(q)^2](t)-\mathcal{E}[V_0(q)V(q)](t),$$

which can be integrated $E_{\rm kin}(t)=E_{\rm total}-E_{\rm init}(t)-E_{\rm coll}(t)$.
For the classical limit $\frac{E_{\rm coll}(t)}{nT}=-\frac{\sqrt3\Gamma^{3/2}}{4x}\partial_y(y\mathcal{F}(y))_{y=x\tau}$, where $\mathcal{F}(y)=1-e^{y^2}{\rm erfc}(y)$ and $\tau=t\omega_p/\sqrt2$
Initial correlations

$$\frac{E_{\rm init}(t)}{nT}=-\frac{\sqrt3\Gamma^{3/2}}{2(x_0^2-x^2)}\left[x\mathcal{F}(x\tau)-x_0\mathcal{F}(x_0\tau)\right],$$

the long time limit of leading to $\frac{E_{\rm total}}{nT}=\frac{\sqrt3\Gamma^{3/2}}{2(x+x_0)}$.



[[4] Simulation: G. Zwicknagel]

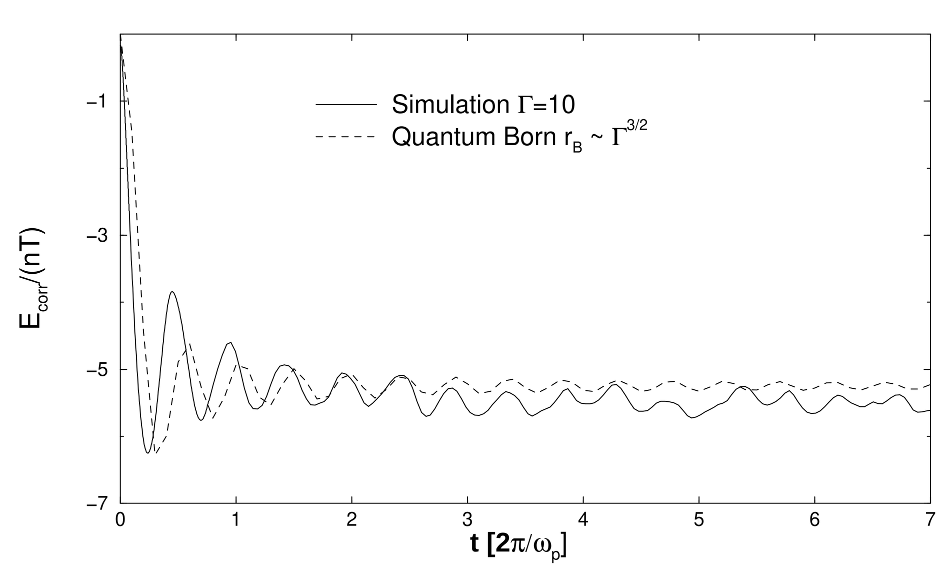
Dense classical OCP by quantum Born

Quantum-Born approximation at low temperatures [2,3]:

$$\frac{E^T_{\rm corr}(t)-E^0_{\rm corr}(t)}{nT}=\frac{1}{(36\pi^4)^{1/6}}\frac{{r_s}^3}{\Gamma}\left(\frac{\sin y\tau}{y\tau}-1\right)\left(\frac{1}{b_l}\arctan(\frac{1}{b_l})+\frac{1}{b_l^2+b_l^4}\right)$$

Bruckner parameter $r_s=\frac{d}{a_B}$, $b_l=\frac{\hbar\kappa}{2p_f}=\sqrt\Gamma(48\pi^2)^{-1/6}$, time in plasma periods $\tau=\frac{2\pi}{\omega_p}t$ or $y\tau=4\epsilon_f t/\hbar=(2)^{4/3}\pi^{5/3}3^{5/6}\tau/\sqrt{r_s}$

Simulation of dense classical plasma [G. Zwicknagel]



best fit ($\hbar\sim T$)

$$r_s^{\rm fit}=\frac{1}{2}\sqrt{\frac{3}{8}}\Gamma^{3/2}$$
$$\lambda^2=\frac{d}{\kappa}=\frac{d^2}{(3\Gamma)^{1/2}}\approx d^2$$

Summary

1. Initial correlations induce a current and energy contribution
2. Classical N particle partition function can be represented by a quantum N-1 particle Eigenwert problem [8]
3. Quantum potentials can be derived which describe classically quantum effects (Kelbg, 3-particle corrections)
4. Oppositely quantum Born results can be used to describe dense classical systems $\Gamma\sim 1..10$ by properly replacing quantum parameter $\lambda\to d$ or $r_s\to\Gamma^{3/2}/4$
5. Test: formation time of correlations by kinetic theory and moleculardynamical simulations
   - low temperature value is universal; ratio $\hbar$ to Fermi energy corresponds to the formation time of quasiparticles [2,3]
   - high temperature limit shows roughly a time scale a particle needs to travel through the potential range (inverse plasma frequency)
   - dynamical result approaches Debye Hückel, while static leads to half the result [6]
   - quantum-Born results describe time evolution of dense classical system replacing $\lambda\to d$ or $r_s\to\Gamma^{3/2}/4$ [8]