Dynamical local fields for quasiparticles

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MAX-PLANCK-GESELLSCHAFT

Outline

- Local field corrections and sum rules
- Problem: third order frequency and compressibility sum rule not simultaneously fulfilled by local field (solution: effective mass)
- General response function for quasiparticle picture
- Response with effective mass and energy shift
- Collisional narrowing
- Comparison with Monte Carlo

Local Field Corrections

Density response function $\delta n(q,\omega)=\chi(q,\omega)V^{\rm ext}(q,\omega)$

Polarisation $\delta n(q,\omega)=\Pi(q,\omega)\delta V^{\rm ind}(q,\omega)$

Induced potential sum of external and local field $(V_q+f_q(\omega))\delta n$

$$\chi(\omega)=\frac{\Pi(\omega)}{1-(V_q+f_q(\omega))\Pi(\omega)}$$

Hubbard'57: $G_H = -\frac{f_q}{V_q}=\frac{1}{2}\frac{q^2}{q^2+k_f^2}$

Singwi et al '68: $G_{STLS} = -\frac{1}{n}\int\frac{dk}{(2\pi)^3}\frac{(k\cdot q)}{k^2}(S_{k-q}-1)$

Further progress: Demanding sum rules Puff'65

$$\begin{aligned}\int\frac{d\omega}{\pi}\omega{\rm Im}\chi(\omega) &= \frac{nq^2}{m}\\ \int\frac{d\omega}{\pi}\omega^3{\rm Im}\chi(\omega) &= 2E_{int}\frac{q^4}{m^2}+\frac{nq^6}{4m^3}-\frac{n^2q^4}{m^2}V_q(I(q)-1)\\ I(q) &= -\frac{1}{n}\int\frac{dk}{(2\pi)^3}(S_{k-q}-S_k)\frac{(k\cdot q)^2V_k}{q^4\,V_q}\end{aligned}$$

Pathak and Vashishta '73, : $G_{PV} = I(q)$

Iwamoto, Krotscheck, Pines '84, : $G_{PV}+\Delta E = I(q)+\frac{2}{nV_q}(E-E_{int})$

Problem

Vaishya, Gupta '73: Local field does not fulfill simultaneously 3. order sum rule and compressibility:

$$nTK=\lim_{q\to 0}S_q=\lim_{q\to 0}\int\frac{d\omega}{n\pi}\frac{1}{1-{\rm e}^{-\beta\omega}}{\rm Im}\chi(\omega,q)$$

Solution: Effective mass

For quasiparticle picture $F(p)=({\rm e}^{\beta(\frac{p^2}{2m(n)}+\Delta(n)-\mu)}+1)^{-1}$

Compressibility should look like $K_0=\frac{\beta}{n^2}\int\frac{dp}{(2\pi)^3}F(p)(1-F(p))$

$$\begin{aligned}K &= \frac{1}{n^2}\frac{\partial n}{\partial\mu}=-\frac{\beta}{n^2}\int\frac{dp}{(2\pi)^3}F(p)(1-F(p))\left([\Delta'(n)-\frac{p^2}{2m}(\ln m)']\frac{\partial n}{\partial\mu}-1\right)\\ &= \frac{K_0}{1+n^2\frac{\delta}{\delta n}\Delta K_0-\frac{3}{2}\frac{\partial\ln m}{\partial\ln n}}\end{aligned}$$

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Response function for interacting quantum liquids

Quantum kinetic equation $\dot{\hat\rho}+i[\hat{\mathcal{E}}+\hat V^{\rm ext},\hat\rho]=\frac{\hat\rho^{\rm l.e.}-\hat\rho}{\tau}$

quasiparticle (Skyrme) energy ε

$$\begin{aligned}\mathcal{E}(\mathbf{p},\mathbf{R},t) &= \sum_q {\rm e}^{i\mathbf{qR}}\langle p+\frac{q}{2}|\hat{\mathcal{E}}|-p+\frac{q}{2}\rangle\\ &\equiv \nabla\left(\frac{1}{2m}-\epsilon_1(n)\right)\nabla+\epsilon_2 n+\epsilon_1[2mE-\frac{1}{i}(\nabla\mathbf{U}+\mathbf{U}\nabla)]+\epsilon_3\nabla^2 n+\epsilon_4 n^\alpha\end{aligned}$$

Relaxation towards local equilibrium

$$f^{\rm l.e.}(\mathbf{p},\mathbf{R},t) = f_0\left(\frac{\varepsilon_0(\mathbf{p}-\mathbf{Q}-\delta\mathbf{Q}(\mathbf{R},t))-\mu-\delta\mu(\mathbf{R},t)}{T+\delta T(\mathbf{R},t)}\right)$$

determined by conservation laws $\sum_p\begin{pmatrix}1\\ \mathbf{p}\\ \varepsilon\end{pmatrix}(f-f^{\rm l.e.})=0$

to obtain $\delta\phi=\sum_p\phi(f-f^{\rm l.e.}+f^{\rm l.e.}-f_0)=\sum_p\phi(f^{\rm l.e.}-f_0)$

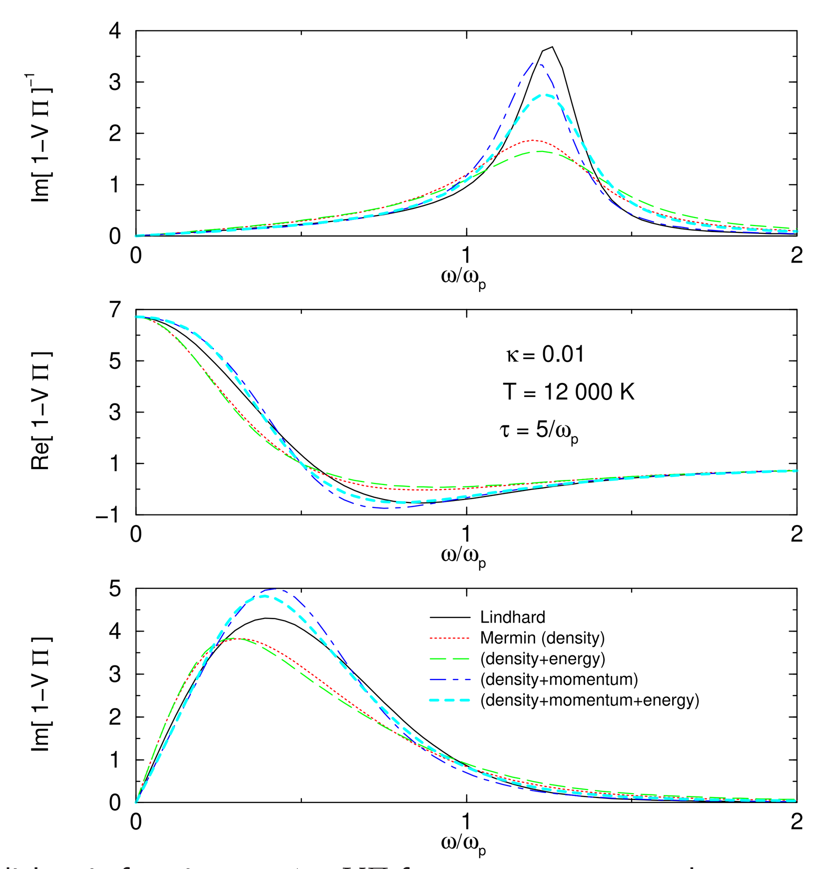
$$\begin{pmatrix}\delta n\\ \delta U_q\\ \delta E\end{pmatrix}=\mathcal{A}[g_\phi]\begin{pmatrix}\delta\mu\\ \delta Q\\ \delta T\end{pmatrix}$$

from linearised kinetic equation

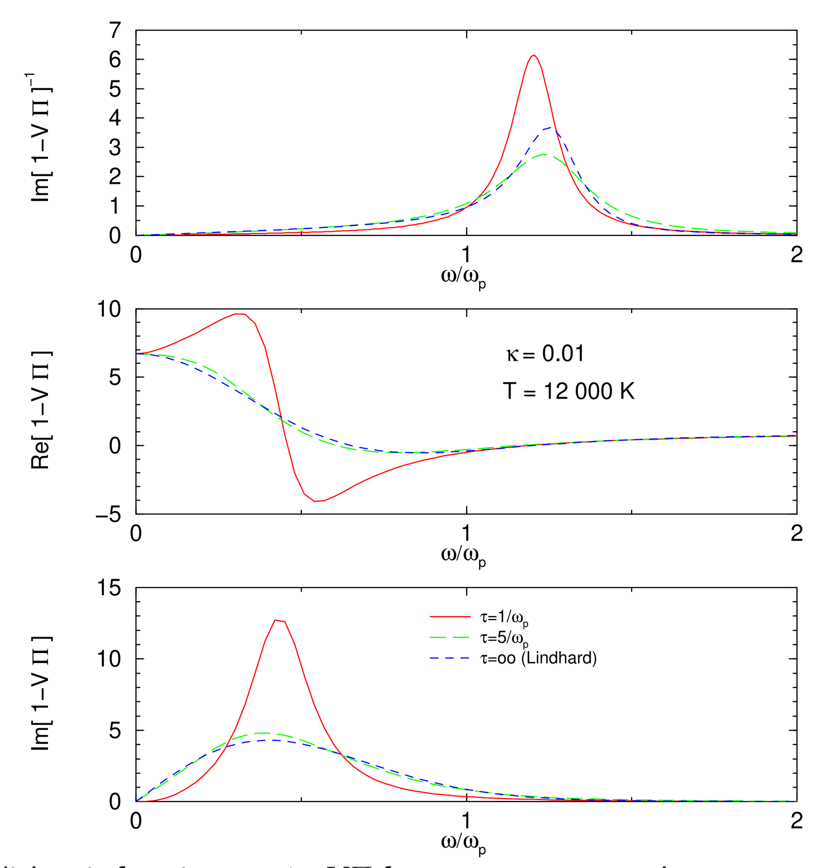
$$\mathcal{I}\begin{pmatrix}\delta n\\ \delta U_q\\ \delta E\end{pmatrix}=\mathcal{B}[g_\phi]\begin{pmatrix}\delta\mu\\ \delta Q\\ \delta T\end{pmatrix}+\mathcal{V}[g_\phi]\begin{pmatrix}\delta n\\ \delta U_q\\ \delta E\end{pmatrix}+\begin{pmatrix}g_1\\ g_{\mathbf{pq}}\\ g_\epsilon\end{pmatrix}V^{\rm ext}$$

$$\boxed{\begin{pmatrix}\delta n\\ \delta U_q\\ \delta E\end{pmatrix}=(\mathcal{I}-\mathcal{V}_g-\mathcal{B}_g\mathcal{A}_g^{-1})^{-1}\begin{pmatrix}g_1\\ g_{\mathbf{pq}}\\ g_\epsilon\end{pmatrix}V^{\rm ext}}$$

Results



The dielectric function $\varepsilon=1-V\Pi$ for a one component plasma system in different approximations. The inverse Debye length is $\kappa^2=\frac{4\pi ne^2}{T}$ and the energy scaled in plasma frequencies $\omega_p^2=\kappa^2T/m$. The relaxation time was chosen arbitrarily as $\tau=5/\omega_p$ and the wave vector $q=0.384\kappa$. The upper most panel shows the excitation function (imag. part of response function).



The dielectric function $\varepsilon=1-V\Pi$ for a one component plasma system with the inclusion of density, momentum and energy conservation for different relaxation times. Collisional narrowing (resonance) if $\omega_p\tau\sim 1$.

Quasiparticle approximation

$$\hat{\mathcal{E}}=-\nabla(\frac{1}{m(\hat n)})\nabla+\Delta(\hat n)$$

$$\chi=\frac{\Pi^{\rm n,j,E}}{1-(\frac{\partial\Delta}{\partial n}+\frac{1}{2nm}\frac{\partial\ln m}{\partial\ln n}\frac{q^2}{4})\Pi^{\rm n,j,E}+\frac{1}{n}\frac{\partial\ln m}{\partial\ln n}\Pi_{13}}$$

where

$$\Pi_{13} = \frac{\Pi^{\rm n,j,E}}{2m}\;\frac{\Pi_h\Pi_2(0)-i\tau\omega\Pi_2(\omega+\frac{i}{\tau})}{\Pi_h\Pi_0(0)-i\tau\omega\Pi_0(\omega+\frac{i}{\tau})}$$

$$\Pi_h = \frac{\Pi_2^2(\omega+\frac{i}{\tau})-\Pi_0(\omega+\frac{i}{\tau})\Pi_4(\omega+\frac{i}{\tau})}{\Pi_2^2(0)-\Pi_0(0)\Pi_4(0)}$$

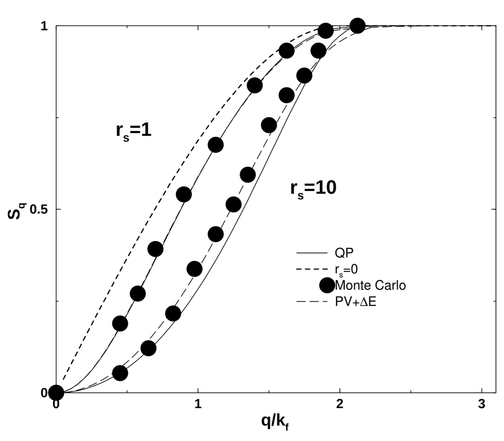
1. Compressibility

$$\frac{n}{\beta}K = \lim_{q\to 0}S(q)=\frac{1}{n\beta}\frac{n^2K_0}{1+n^2K_0\frac{\partial\Delta}{\partial n}-\frac{3}{2}\frac{\partial\ln m}{\partial\ln n}}$$

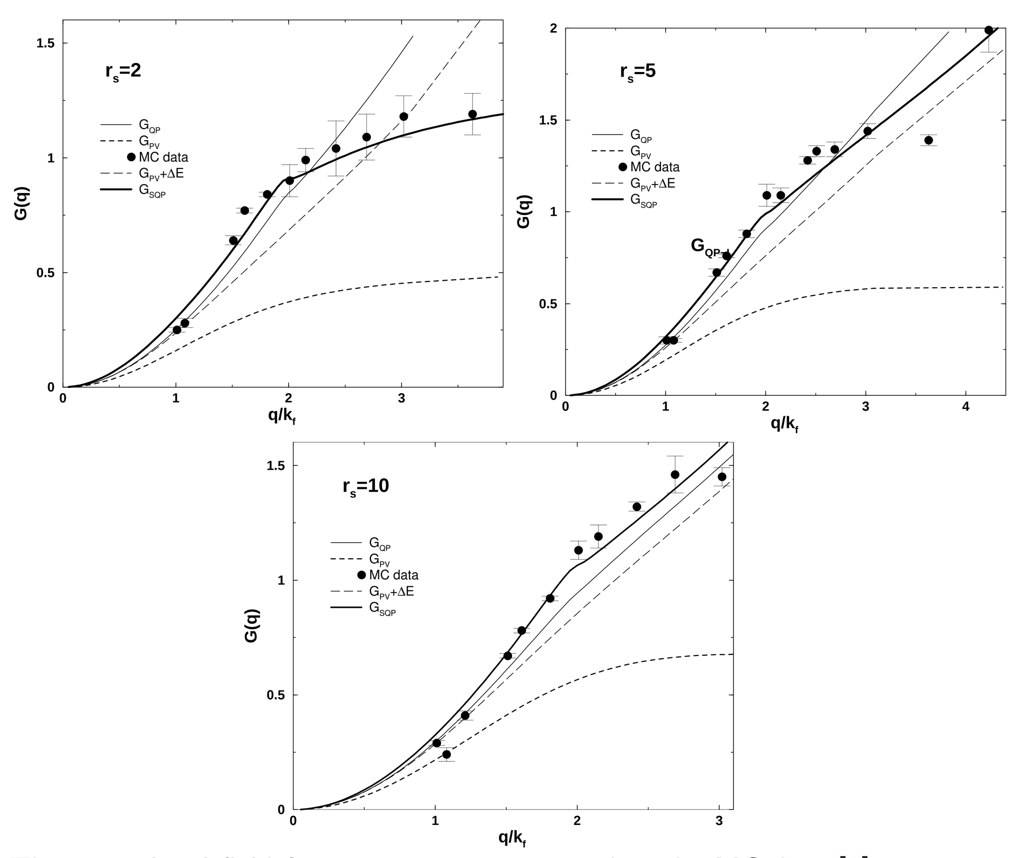
2. Third order sum rule

$$\boxed{V_q(I(q)-1)=\frac{1}{2mn}\left(\frac{\Pi_2(0)}{\Pi_0(0)}-\frac{q^2}{4}\right)\frac{\partial\ln m}{\partial\ln n}-\frac{\delta\Delta}{\delta n}+\Delta E}$$

T=0 Electrongas



The static structure factor for $r_s=1$ and $r_s=10$ from the Pathak and Vashishta (PV)-, the (PV+ΔE)-, the quasiparticle (QP)- and selfconsistent quasiparticle (SQP) model compared to the MC data [8] presented in [10].



The static local field for $r_s=2,5,10$ compared to the MC data [9].

Summary

- Response function for general quasiparticle parametrization derived
- Energy, density and momentum conserving relaxation time approximation
- Momentum conservation corresponds to additional dynamical local field

$$\frac{1}{\Pi^{\rm n,j,E}(\omega)}-\frac{1}{\Pi^{\rm n,E}(\omega)}=\frac{1}{\Pi^{\rm n,j}(\omega)}-\frac{1}{\Pi^{\rm n}(\omega)}=-\frac{i\omega\,m}{\tau\,nq^2}$$

- Effective mass and energy allows to fulfill third order frequency and compressibility sum rule simultaneously
- If collision frequency $\sim$ collective mode: Collisional narrowing
- Improved description of Monte Carlo data

r_s	γ_0 MC	δ MC	$1-g(0)$ MC	$1-g(0)$ SQP	$1-g(0)$ QP	$1-g(0)$ PV+ΔE
1	0.2567	0.036	0.7276	0.7240	0.6626	0.6971
2		0.091	(0.8627)	0.8627	0.7666	0.8346
3	0.2722		0.9078	0.9201	0.8456	
5	0.2850	0.292	0.9768	0.9627	0.9351	1.0558
10	0.3079	0.619	0.9976	0.9733	0.9613	1.1231

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