Ab Initio Plasmon Dispersion of the Warm Dense Electron Gas

Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät

Paul Hamann [1*], Tobias Dornheim [2], Jan Vorberger [3], Zhandos Moldabekov [4] and Michael Bonitz [1]
[1] CAU Kiel, Germany; [2] CASUS, Germany; [3] HZDR, Germany, [4] Al-Farabi Kazakh National University

Abstract

The plasmon dispersion $\omega(q)$ and damping $\gamma(q)$ contain important information on the state of warm dense matter. On the other hand, x-ray Thomson scattering (XRTS) experiments provide accurate data for the dynamic structure factor $S(q,\omega)$ that is directly linked to the plasmon spectrum [1]. However, details of this link depend on the quality of the theoretical model for the dielectric function. Here we present the first ab initio data for the dielectric function that is obtained by quantum Monte Carlo simulations [2]. This allows us to obtain high quality results for $\omega(q)$ and $\gamma(q)$ of the electron component at warm dense matter conditions that differ significantly from previous models. Second, we critically analyze the commonly used weak damping approximation for the dispersion and improve it by performing the analytic continuation of the retarded dielectric function. This yields results that apply at strong damping and large wave numbers as well, which is the basis for a more accurate comparison with XRTS experiments [3].

PIMC approach to the dielectric function

- Evaluate imaginary-time density autocorrelation function

$$F(q,\tau) = \frac{1}{N}\langle \hat\rho(q,\tau)\hat\rho(-q,0)\rangle \,. \tag{1}$$

- Obtain dynamic structure factor

$$F(q,\tau) = \int_{-\infty}^{\infty} \mathrm{d}\omega\, S(q,\omega) e^{-\tau\omega} \tag{2}$$

by stochastically sampling dynamic local field correction $G(\boldsymbol{q},\omega)$:

$$\chi(\boldsymbol{q},\omega) = \frac{\chi_0(\boldsymbol{q},\omega)}{1 - v_{\boldsymbol{q}}\left[1 - G(\boldsymbol{q},\omega)\right]\chi_0(\boldsymbol{q},\omega)}, \tag{3}$$

where

$$S(\boldsymbol{q},\omega) = -\frac{\operatorname{Im}\chi(\boldsymbol{q},\omega)}{\pi n\left(1 - e^{-\beta\omega}\right)}, \tag{4}$$

incorporating additional constraints on $G(\boldsymbol{q},\omega)$. [2]

- Limit $\omega \to 0$ can be obtained directly:

$$\chi(\boldsymbol{q}) = -n\int_0^{\beta} \mathrm{d}\tau\, F(\boldsymbol{q},\tau). \tag{5}$$

Static LFC $G(\boldsymbol{q}) = G(\boldsymbol{q},0)$ sufficient description for $r_s \lesssim 4$.

- Calculate related quantities, e.g. dielectric function. [4]

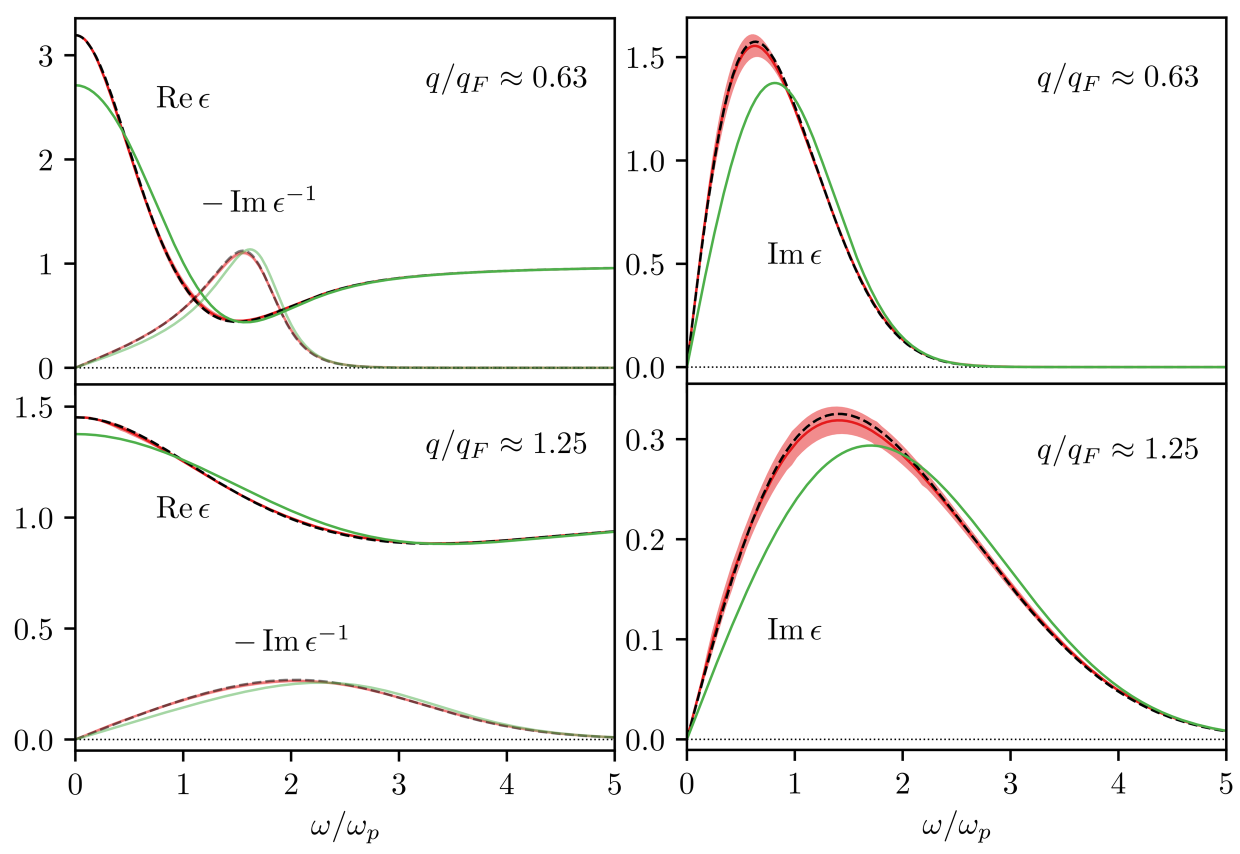

FIG. 1: Dielectric function for $r_s = 2$ and $\theta = 1$. Green: RPA, black (red): PIMC results using static (dynamic) LFC.

Collective excitations (Plasmons)

- In an isotropic medium, existence of longitudinal collective plasma oscillation follows from the roots of the longitudinal dielectric function:

$$\epsilon[\hat\omega(q), q] = 0\,, \tag{6}$$

where $\hat\omega(q)$ is the plasmon frequency for wavenumber q which is, in general, a complex function. [5]

- Undampened solutions exist only at zero temperature, in thermodynamic equilibrium, solutions $E(q,t) \sim e^{-i\hat\omega(q)t}$ vanish in long time limit, $\operatorname{Im}\hat\omega(q) < 0$.
- Weak damping: approximate solution by roots of the real part, damping $\gamma(q) = -\operatorname{Im}\hat\omega$ follows in perturbation theory,

$$0 = \operatorname{Re}\epsilon[\omega(q), q], \tag{7}$$

$$\gamma(q) = \frac{\operatorname{Im}\epsilon[\omega(q),q]}{\frac{\partial}{\partial\omega}\operatorname{Re}\epsilon[\omega(q),q]}\,, \quad |\gamma(q)| \ll \omega(q)\,. \tag{8}$$

Results can be extended to higher order terms, approximation still limited to q-range where roots of Re $\epsilon(q,\omega)$ exist.

Analytic continuation of $\epsilon(\boldsymbol{q},\omega)$

- On the real frequency axis, solutions of Re $\epsilon = 0$ vanish at relatively small wave numbers, making it impossible to apply the weak damping approximation.
- Instead, look for full solutions of Eq. (6) at complex frequencies $z = \omega(q) - i\gamma(q)$:

$$E(q,t) \sim e^{i\omega(q)t}e^{-\gamma(q)t} \tag{9}$$

- Retarded/advanced RPA polarization function:

$$\Pi^{R/A}(\boldsymbol{q},z) = \int \frac{d\boldsymbol{p}}{(2\pi)^3}\frac{f(E_{\boldsymbol{p}}) - f(E_{\boldsymbol{p}+\boldsymbol{q}})}{E_{\boldsymbol{p}} - E_{\boldsymbol{p}+\boldsymbol{q}} + z}\,, \tag{10}$$

- Retarded function in lower half-plane:

$$\tilde\Pi^R(\boldsymbol{q},z) = \Pi^A(\boldsymbol{q},z) - 2\pi i\,\hat\Pi(\boldsymbol{q},z)\,. \tag{11}$$

where

$$\begin{aligned}\hat\Pi(\boldsymbol{q},\omega) &= \frac{1}{i}\left\{\Pi^R(\boldsymbol{q},\omega+i\delta) - \Pi^A(\boldsymbol{q},\omega-i\delta)\right\}\\ &= \int\frac{d\boldsymbol{p}}{(2\pi)^3}\left\{f\left(E_{\boldsymbol{p}}\right) - f\left(E_{\boldsymbol{p}+\boldsymbol{q}}\right)\right\}\\ &\quad\times\delta\left[\omega + E_{\boldsymbol{p}} - E_{\boldsymbol{p}+\boldsymbol{q}}\right]\,,\end{aligned} \tag{12}$$

- Dielectric function including correlations via static LFC $G(\boldsymbol{q})$,

$$\epsilon^R(\boldsymbol{q},z) = 1 - \frac{v_{\boldsymbol{q}}\tilde\Pi^R(\boldsymbol{q},z)}{1 + v_{\boldsymbol{q}}G(\boldsymbol{q})\tilde\Pi^R(\boldsymbol{q},z)} \tag{13}$$

Choosing $G(\boldsymbol{q}) = 0$ recovers the RPA.

- Collective modes can still be identified at higher wave numbers (Fig. 2, Fig. 3).
- Obtain results for plasmon dispersion and damping

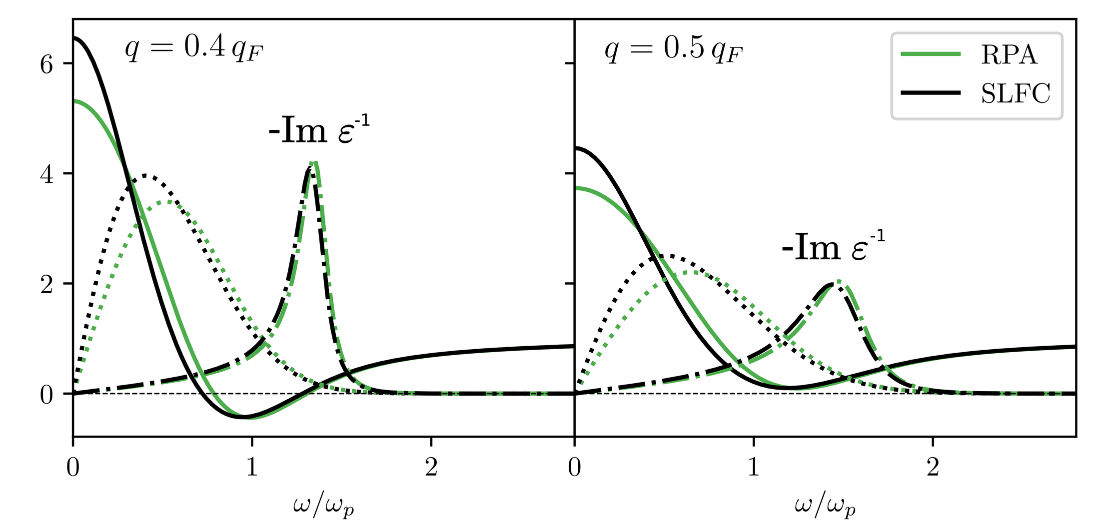

FIG. 2: Real and imaginary part of the dielectric function for $r_s = 2$ and $\theta = 1$. Left: peak in -Im ϵ^{-1} (resembling DSF) in vicinity of root where Im ϵ is small. Solutions of Re $\epsilon(q,\omega) = 0$ vanish at higher wave-numbers (right).

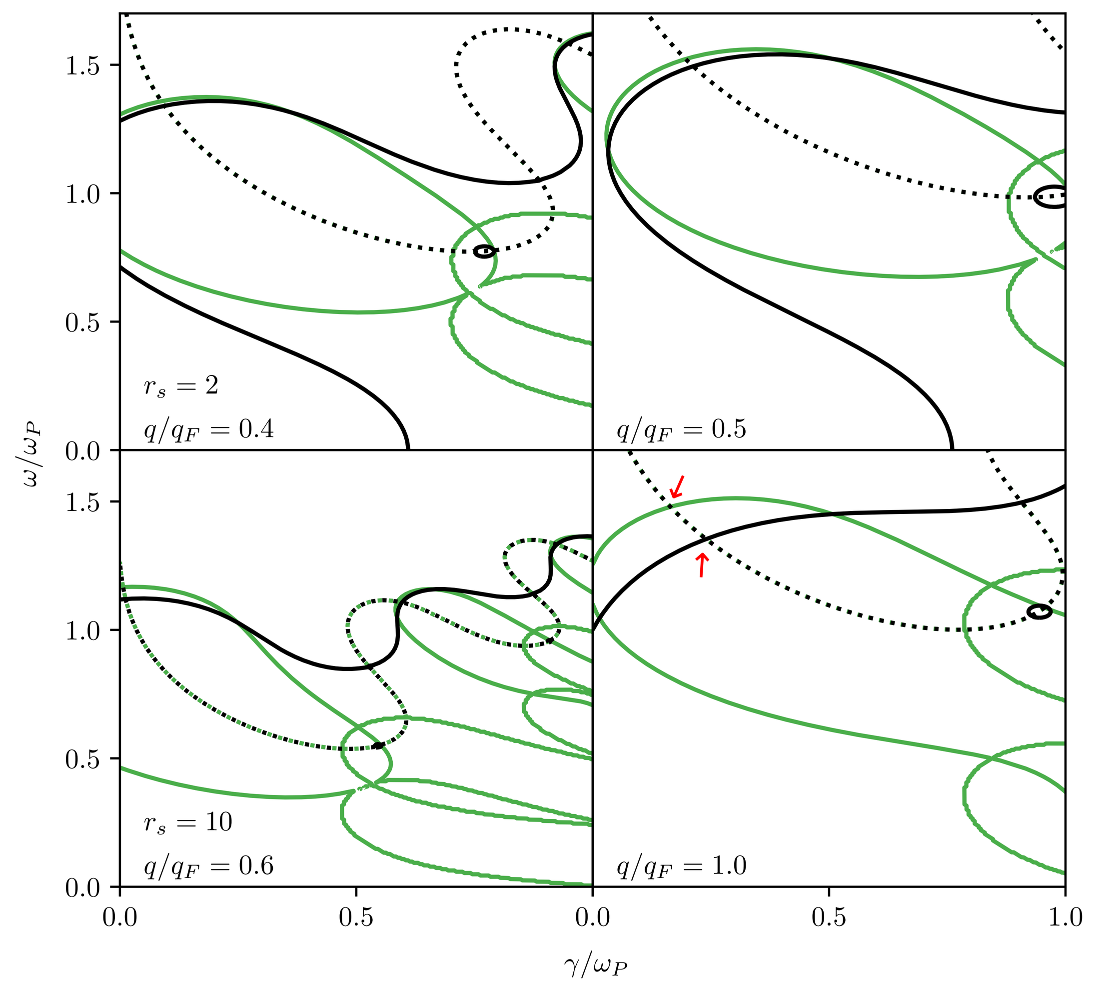

FIG. 3: Dielectric function in the complex plane. $\theta = 1$ Solid lines: Re $\epsilon = 0$, dotted: Im $\epsilon = 0$. Plasmon frequency and damping can be identified from the intersections (red arrows).

Results

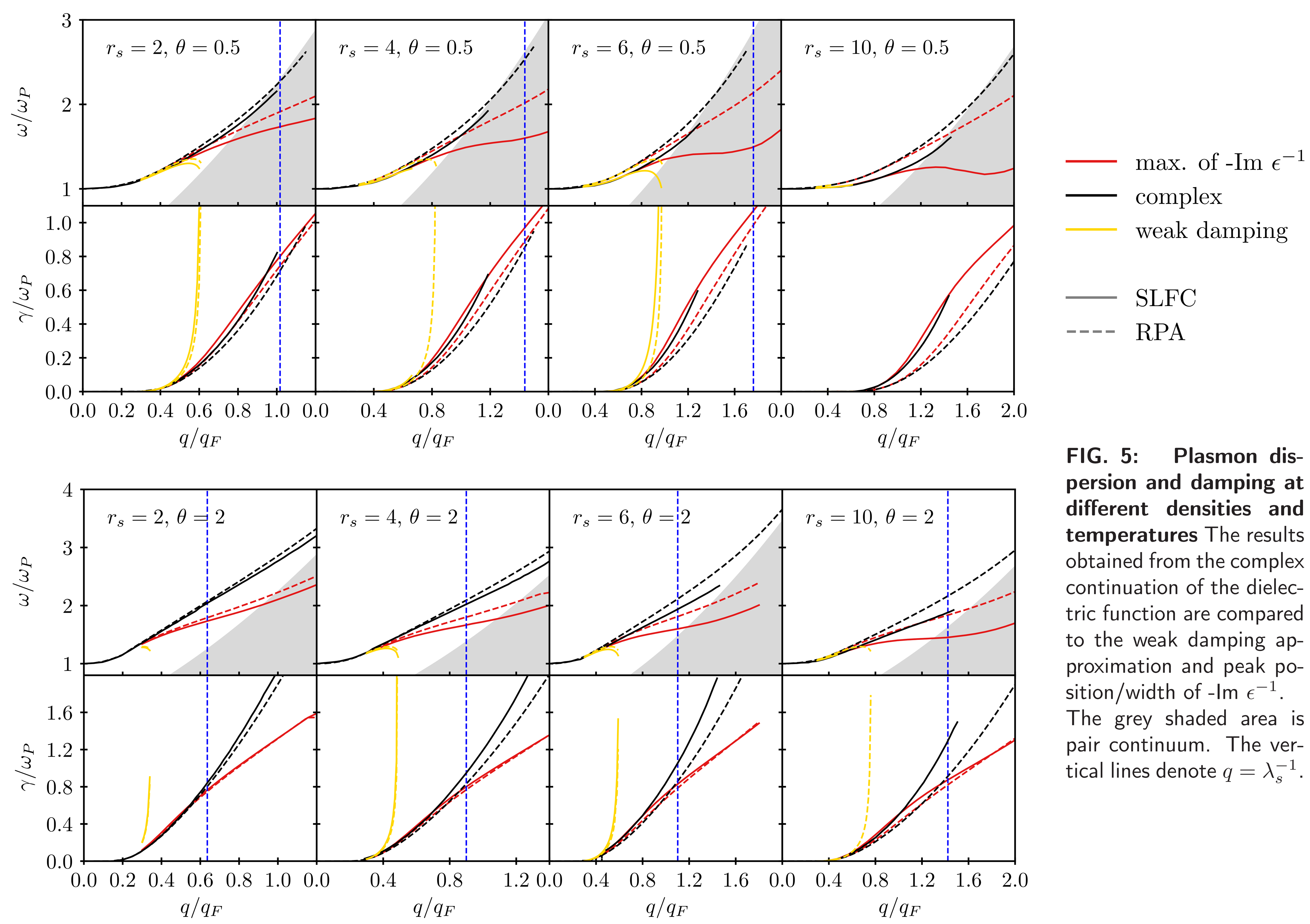

FIG. 5: Plasmon dispersion and damping at different densities and temperatures The results obtained from the complex continuation of the dielectric function are compared to the weak damping approximation and peak position/width of -Im ϵ^{-1}. The grey shaded area is pair continuum. The vertical lines denote $q = \lambda_s^{-1}$.

Conclusion and Outlook

- Weak damping approximation is only accurate for very small wave numbers.
- Location and width of peak in spectral function $S \sim$ -Im ϵ^{-1} start to deviate from complex dispersion relation with increasing q.
- Considering the true plasmon dispersion in the complex plane allows to distinguish collective and single-particle contributions to the dynamic structure factor.

Literature

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* Paul Hamann • Christian-Albrechts-Universität Kiel • Leibnizstr. 15, 24098 Kiel, Germany • phamann@physik.uni-kiel.de