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Dynamic pair excitations in 2D Fermi fluids

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Abstract
We apply a theory (Böhm *et al* 2006 *AIP Conf. Proc.* **850** 111, 2007 *Int. J. Mod. Phys.* B **21** 2055) developed recently on dynamic two-pair fluctuations to layered systems, such as electrons in semiconductor hetero-structures or ^{3}He on graphite. The theory fulfils the zeroth and first frequency moment sum rule. Results are presented for the static effective particle–hole interaction, the dynamic structure function and the dispersion of the plasmon.

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1. Motivation

Two-dimensional (2D) systems show more pronounced correlation effects than the bulk: the particles have fewer possibilities to 'evade' and to screen the interaction. It is worthwhile to apply the dynamic theory developed recently [1] for fermions to layers of N electrons or ^{3}He atoms (with an area density n). A common paradigm is to use a generalized random phase approximation (RPA) form for the density response function

$$\chi(q,\omega) = \chi^0(q,\omega)/[1 - V^{\text{eff}}(q)\chi^0(q,\omega)]. \tag{1}$$

In charged systems for the effective static interaction, commonly $V^{\text{eff}} =: (1-\mathcal{G})v^{\text{C}}$ with $v^{\text{C}}(q) = 2n\pi \text{e}^2/q$ is used [3]. By including dynamic pair fluctuations our approach improves both the numerator and the denominator of (1) (we refer to [2] for details)

$$\chi(q,\omega) = \chi^s(q,\omega)/[1 - V^{\text{eff}}(q)\chi^s(q,\omega) - \Lambda(q,\omega)]. \tag{2}$$

In general, V^{eff} in (1) is the dynamic irreducible interaction in the particle–hole channel. Summing all parquet diagrams in a static local approximation yields the 'correlated' RPA (cRPA), where $V^{\text{eff}}(q)$ is determined by the (free) static structure factor $S_{(\text{F})}(q)$

$$V^{\text{eff}}(q) \to V_{\text{ph}}(q) = \frac{\hbar^2 q^2}{4m}\left[\frac{1}{S^2(q)} - \frac{1}{S_{\text{F}}^2(q)}\right]. \tag{3}$$

Not surprisingly, different sum-rules (SRs) for χ lead to mutually exclusive conditions [3] for a *single* static function $V^{\text{eff}}(q)$; equation (3) is designed to fulfil the ω^0-SR, but it violates the $\omega = 0$ requirements [3, 4]. This is corrected by including dynamic pair fluctuations.

Measurements of the dynamic structure factor $S(q,\omega)$ of ^{3}He films [1] yield another compelling argument for our approach: the collective mode is found *inside* a broad continuum, not explicable with (1). An effective mass may move the theoretical value toward the experimental one; however, it also shifts the particle–hole (1ph) continuum to stay *below*. Either the phonon–roton is inside the 1ph continuum or the experiments show a broad multi-particle continuum. *Both* effects are contained in our approach.

For 2D electrons, a most advanced dynamic theory was developed by Neilson *et al* [5]. Invoking the 'self' motion γ^s of the exchange-correlation hole they proposed

$$\chi(q,\omega) = \frac{\widetilde{\chi}^s(q,\omega)}{1 - \widetilde{V}^{\text{eff}}(q)\widetilde{\chi}^s(q,\omega) - \frac{m\omega}{\hbar q^2}[\gamma(q,\omega) - \gamma^s(q,\omega)]}. \tag{4}$$

$\widetilde{\chi}^s(q,\omega) = \chi^0(q,\omega - \gamma^s)$ is the Lindhard function at a frequency shifted due to the self-motion. Using $\bar{v} = v^{\text{STLS}}$ (cf (19) of [5]) and $-\mathbf{q}'' = \mathbf{q} + \mathbf{q}'$, the memory function γ reads

$$\begin{aligned} \frac{m\omega}{\hbar q^2}\gamma(q,\omega) &= \frac{1}{2N}\sum_{\mathbf{q}'} |Y_{q,q',q''}|^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'\,\mathrm{d}\omega''}{N^2} \frac{S(q',\omega')S(q'',\omega''-\omega')}{(\omega-\omega'')\omega''} \\ Y_{q,q',q''} &= \left(\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}v^{\text{STLS}}(q') + \frac{\mathbf{q}\cdot\mathbf{q}''}{q^2}v^{\text{STLS}}(q'')\right). \end{aligned} \tag{5}$$

In each self-consistency step in solving (4)–(5), the static interaction $\widetilde{V}^{\text{eff}}(q)$ is adjusted so that the static $S(q)$ obtained from Im χ remains unchanged and coincides with that of Monte Carlo (MC, [6]). If the rhs of (5) is simplified by using the plasmon-pole-approximation $S(q,\omega) \approx NS(q)\delta(\hbar\omega - \varepsilon(q))$ with $\varepsilon(q) = \hbar^2q^2/2mS(q)$, one arrives at

$$\frac{m\omega}{\hbar q^2}\gamma(q,\omega) \approx \frac{1}{2N}\sum_{\mathbf{q}'} |Y_{q,q',q''}|^2 \frac{S(q')S(q'')}{\hbar\omega - \varepsilon(q') - \varepsilon(q'')} \frac{\omega}{\varepsilon(q') + \varepsilon(q'')}. \tag{6}$$

We compare this to the theory containing dynamic pair correlations for charged bosons [7], where $\chi(q,\omega > 0) = S(q)/[\hbar\omega - \varepsilon(q) - \Sigma(q,\omega)]$. The self-energy Σ has the same poles as (6); using the direct correlation function X and omitting static triplet fluctuations

$$\Sigma(q,\omega) = \frac{1}{2NS(q)}\sum_{\mathbf{q}'} \left|\frac{\hbar^2\mathbf{q}\cdot\mathbf{q}'}{2m}X(q') + \frac{\hbar^2\mathbf{q}\cdot\mathbf{q}''}{2m}X(q'')\right|^2 \frac{S(q')S(q'')}{\hbar\omega - \varepsilon(q') - \varepsilon(q'')}. \tag{7}$$

The main difference is the specific vertex $Y_{q,q',q''}$ and a renormalization of the Feynman energies in the self-consistent treatment. The bosonic theory [7, 8] very successfully improved the prediction for the ^{4}He spectrum compared to the cRPA.

2. Dynamic pair theory

In deriving our fermionic theory [1] we therefore closely followed that for bosons. As a first step, exchange effects and topologically similar ladder diagrams are neglected, since the physical effects governing the collective mode are expected to be the same in ^{4}He and ^{3}He. Also, with increasing coupling, where correlations get more and more important, the Pauli principle becomes less relevant than interaction effects. Finally, if the exact $S(q)$ is used in $\Sigma(q,\omega)$, exchange is properly accounted for in many static quantities, as our $\chi(q,\omega)$ preserves the ω^0 (as well as the $f-$) sum-rule.

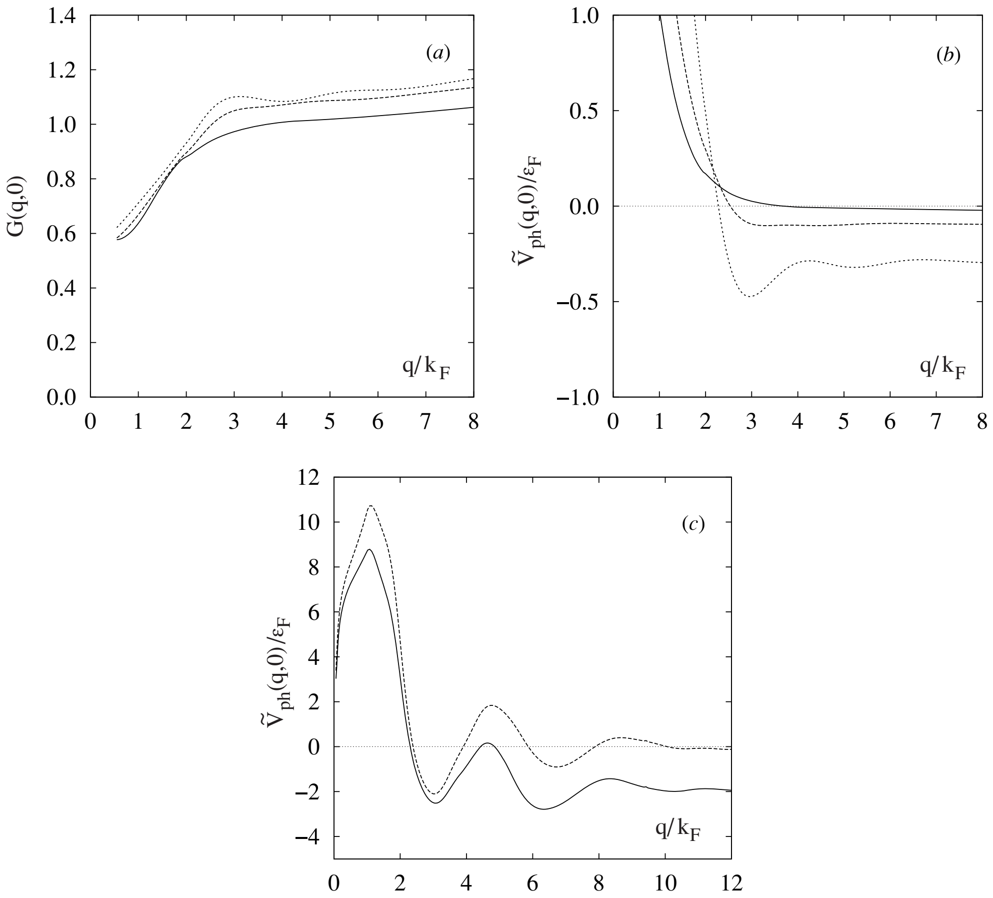

Figure 1. (*a*) Static local field correction and (*b*) static interaction of 2D electrons. The densities correspond to $n^{-1} = \pi a_B^2 r_s^2$ with $r_s = 1, 2$ and 5 (full, dashed and dotted line, respectively). (*c*) Static interaction of 2D ^{3}He for $n = 0.061\text{Å}^{-2}$ within the full theory (solid line) and RPA (dashed).

When possible without losing the essential physics, we replaced the dynamic fluctuations by their Fermi-sea averages, to attain numerically tractable equations. Despite these simplifications the resulting $\chi^s(q,\omega)$ and $\Lambda(q,\omega)$ in (2) are unwieldy. We refer to [2] for the explicit expressions and here prefer to discuss the consequences. Ground-state properties enter our theory via $V_{\text{ph}}(q)$ and $\varepsilon(q)$, where we use $S(q)$ from MC [9]. Since MC cannot yield high accuracy $q \to 0$ data, some caution is in order there. However, x-ray scattering experiments probe large q, where the MC $S(q)$ is excellent and where dynamic correlations are highly relevant.

Of particular interest is the static $\omega = 0$ behavior of the response function, where χ^{cRPA} with V_{ph} (3) is even qualitatively wrong. Figure 1 shows the improved static $\widetilde{V}_{\text{ph}}$

$$\chi(q,\omega=0) := \frac{\chi^0(q,0)}{1-\widetilde{V}_{\text{ph}}(q,0)\chi^0(q,0)} := \frac{\chi^0(q,0)}{1-v^{\text{C}}(q)(1-G(q,0))\chi^0(q,0)} \tag{8}$$

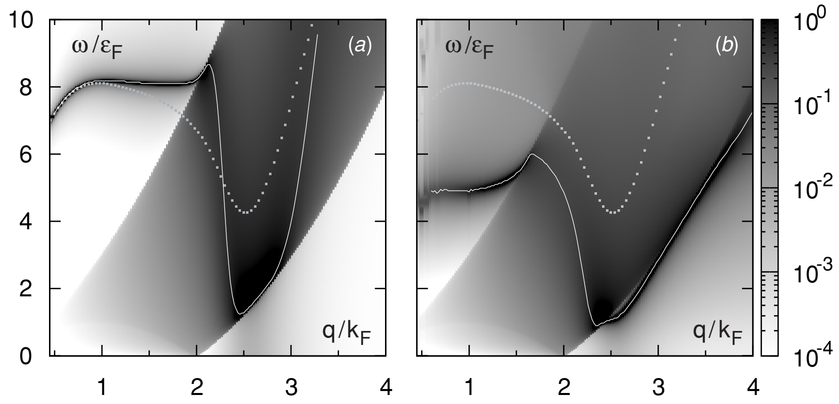

Figure 2. Logarithm of $S(q, \omega)$ for $r_s = 40$ in (a) cRPA and (b) including dynamic pair correlations. The white line gives the main peak, squares the Feynman excitations. (Any cRPA strength outside the 1ph region is due to artificial plasmon broadening).

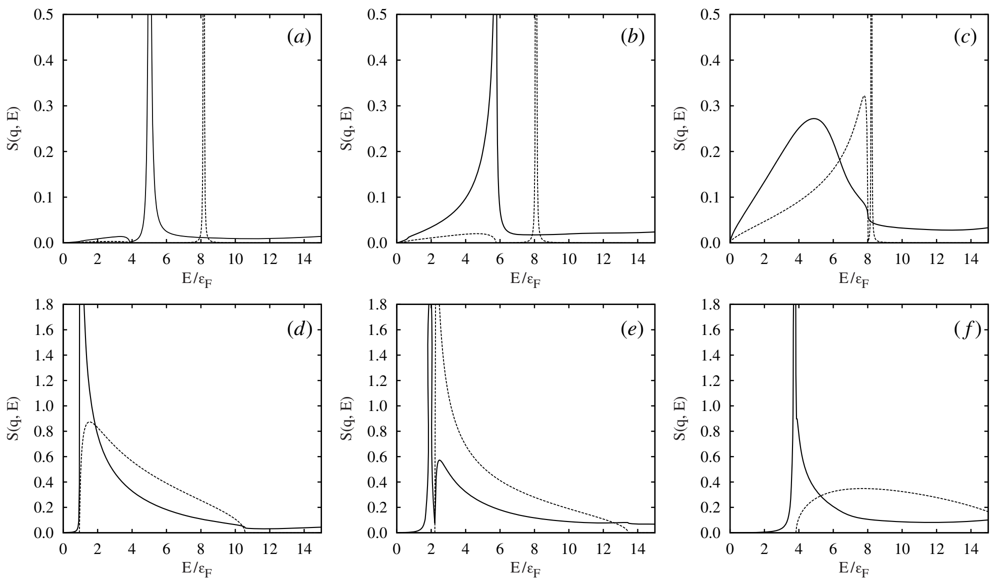

Figure 3. Dynamic structure factor for wave vectors (in Fermi vectors k_F), $q = 1.2, 1.6, 2.0$ (top row, (a)–(c)) and 2.4, 2.8, 3.2 (bottom row, (d)–(f)) at $r_s = 40$. Full line: present theory, dashed line: cRPA (with artificially broadened plasmon).

(contributions result from both, $\chi^s(q, 0)$ and $\Lambda(q, 0)$). As required, $G(q, 0)$ grows linearly with q and $\widetilde{V}_{\mathrm{ph}}(q, 0)$ reaches a finite value, both for electrons and for ^{3}He. The quantitative values are not correct [3, 10], due to the above-mentioned approximations.

Dynamic correlations become important for the plasmon at $r_s \gtrapprox 10$. For comparison with [5] we chose the same r_s (= 40, supercooled liquid) to show in figure 2 the spectrum for $q \geqslant k_F/2$ (below the RPA $\propto \sqrt{q}$ behavior applies). At $q \gtrapprox 2.4k_F$ the plasmon re-emerges from the 1ph continuum on the low energy side and flattens when it reaches twice the Bijl–Feynman 'roton' value; (the correct value requires a renormalization of $\varepsilon(q)$ in (7)). A detailed comparison of the plasmon with and without including two-pair excitations is given in figure 3.

For high ω we predict a significantly lower energy implying a smaller q_c for Landau damping (1.62 instead of 2.05 in cRPA), as well as a distinctly visible low ω mode. Experiments at higher r_s [11] would be highly desirable.

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