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Effective Mass Calculations for Two-dimensional Gas of Dipolar Fermions

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Abstract We consider a two-dimensional system of ultracold dipolar fermions with dipole moments aligned in the perpendicular direction. We use the static structure factor information from Fermi-Hypernetted-Chain calculations to obtain the effective many-body dipole–dipole interaction and calculate the many-body effective mass of the system within the G_0W approximation to the self-energy. A large cancellation between different contributions to the self-energy results in a weak dependence of the effective mass on the interaction strength over a large range of coupling constants.

Keywords Dipole–dipole interaction · Effective mass · G_0W approximation

1 Introduction

The field of ultracold gases has opened up new opportunities to study novel states of matter, which may have promising applications in quantum simulations and quantum computing [1]. In particular, the examination of polar atoms or molecules, due to their long-range and anisotropic dipole–dipole interactions is a good candidate for studying quantum many-body states [2]. This unique interaction results in the emergence of a rich variety of interesting quantum phases [2–4].

Aikawa et al. [5] have directly observed the deformed Fermi surface in dipolar Fermi gases of strongly magnetic Erbium atoms, due to the anisotropic dipole–dipole interaction. The formation of ultracold fermionic $^{23}Na^{40}K$ polar molecules [6] and

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NaLi Feshbach molecules [7] and the observation of the rovibrational ground state in $^{23}Na^{40}K$ molecules have been reported too [8]. First quantum degenerate dipolar Fermi gas of ^{161}Dy atoms with a dipole moment of $\mu = 10\,\mu_B$, where μ_B is the Bohr magneton, has been produced through laser cooling down to $10\,\mu K$ [9]. The creation of a degenerate dipolar Fermi gas of Erbium atoms with large magnetic moment μ of $7\,\mu_B$ by the evaporative cooling method has been reported by Aikawa et al. [10].

Low-energy dynamical properties of dipolar Fermi systems are phenomenologically expressed by using Landau's Fermi-liquid theory [11,12]. Fermi-liquid parameters of dipolar fermions have been studied by several researchers [13–16] in a variety of models and approaches. In these calculations bare interactions, mean-field theory or second-order perturbation theory has been used limiting the applicability to weakly interacting systems.

The purpose of this work is to study the effective mass of a 2D dipolar Fermi gas within the G_0W approximation to the self-energy using better effective interactions in the strongly coupled regime. As the ultracold dipolar gases provide useful model systems to perform standard calculations, we hope our results will shed light on similar systems.

The rest of this paper is organized as follows. In Sect. 2 we introduce our model and give the details of the method we use to calculate the many-body self-energy and the effective mass. In Sect. 3 we illustrate our numeric results for the single-particle spectrum and effective mass. Finally, in Sect. 4, we give a summary and conclude our results.

2 Formalism

We consider a two-dimensional system of atomic or molecular gas of dipolar fermions with their dipole moments aligned in the perpendicular direction. The isotropic dipole–dipole interaction between particles reads

$$v_{\mathrm{dd}}(r) = \frac{C_{\mathrm{dd}}}{4\pi}\frac{1}{r^3}. \tag{1}$$

Here C_{dd} is the dipole–dipole coupling constant, which is d^2/ϵ_0 for molecules with permanent electric dipole d and $\mu_0\mu^2$ for atoms with permanent magnetic dipole μ, where ϵ_0 and μ_0 are the permittivity and permeability of vacuum, respectively. At zero temperature all the properties of this dipolar system will depend on a single dimensionless coupling constant

$$\lambda = k_F r_0, \tag{2}$$

where $r_0 = mC_{\mathrm{dd}}/(4\pi\hbar^2)$ is a characteristic length scale and $k_F = \sqrt{4\pi n}$ is the Fermi wave vector with n being the 2D density. Note that here m is the bare (non-interacting) mass of dipoles, and the system is spin-polarized.

In this paper, we examine the physical effects contributing to the effective mass of a 2D dipolar Fermi liquid. Technically, our approach is similar to the one of Refs. [17–19], performed for liquid ^{3}He. The appropriate quantity for the effective mass is the single-particle Green's function $G(k,\omega)$ in the vicinity of the Fermi surface. It is expressed in terms of the proper self-energy $\Sigma(k,\omega)$ [20]

$$G(k,\omega)=\frac{1}{\hbar\omega-\varepsilon_0(k)-\Sigma(k,\omega)}. \tag{3}$$

Here $\varepsilon_0(k)=\hbar^2k^2/(2m)$ is the non-interacting single-particle spectrum. The physical excitation spectrum is determined by obtaining the poles of the Green's function in the (k,ω) plane. We assume low-lying excitations and resort to the G_0W approximation to calculate the self-energy

$$\begin{aligned}\Sigma(k,E)&=u(k)+i\int\frac{\mathrm{d}^2\mathbf{q}\,\mathrm{d}(\hbar\omega)}{(2\pi)^3}G^0(\mathbf{k}-\mathbf{q},E-\hbar\omega)W^2(q)\chi(q,\omega)\\&=u(k)+\Sigma^{(\rho)}(k,E).\end{aligned} \tag{4}$$

Here the full self-energy is split into two terms: static mean-field term, i.e., "Fock" term $u(k)$ and the dynamic term $\Sigma^{(\rho)}(k,E)$, which originates from the density fluctuations. The Fock term is determined as

$$u(k)=-\int\frac{\mathrm{d}^2\mathbf{q}}{(2\pi)^2}W(\mathbf{k}-\mathbf{q})n_{\mathrm{FD}}(\varepsilon_0(q)). \tag{5}$$

Here $n_{\mathrm{FD}}(\varepsilon)$ is the Fermi–Dirac distribution function, $W(q)$ is the effective dipole–dipole interaction, and $\chi(q,\omega)$ is the density–density linear response function. Within a random-phase approximation (RPA) like mean-field approximations, the density–density response function could be expressed as

$$\chi(q,\omega)=\frac{\chi_0(q,\omega)}{1-W(q)\chi_0(q,\omega)}. \tag{6}$$

The dynamical term of self-energy is easily calculated after Wick rotation in the complex frequency plane. Therefore, this part is divided into two terms: a smooth line-term, with an integral along the imaginary frequency axis, and a pole term originating from the residue of the single-particle Green's function, i.e.,

$$\Sigma^{(\rho)}(k,E)=\Sigma^{(\rho)}_{\mathrm{line}}(k,E)+\Sigma^{(\rho)}_{\mathrm{pole}}(k,E), \tag{7}$$

with

$$\Sigma^{(\rho)}_{\mathrm{line}}(k,E)=-\int\frac{\mathrm{d}^2\mathbf{q}\,\mathrm{d}(\hbar\omega)}{(2\pi)^3}W^2(q)\chi(q,i\omega)\frac{E-\varepsilon_0(|\mathbf{k}-\mathbf{q}|)}{[E-\varepsilon_0(|\mathbf{k}-\mathbf{q}|]^2+(\hbar\omega)^2}, \tag{8}$$

and

$$\begin{aligned}\Sigma^{(\rho)}_{\mathrm{pole}}(k,E)=&\int\frac{\mathrm{d}^2\mathbf{q}}{(2\pi)^2}W^2(q)\chi(q,E-\varepsilon_0(|\mathbf{k}-\mathbf{q}|))\\&\times\left[\Theta(E-\varepsilon_0(|\mathbf{k}-\mathbf{q}|))-\Theta(E_{\mathrm{F}}-\varepsilon_0(|\mathbf{k}-\mathbf{q}|)\right].\end{aligned} \tag{9}$$

Here E_F is the Fermi energy, $\chi(q, i\omega)$ is the density–density response function along the imaginary frequency axis, which could be obtained from Eq. (6) in terms of the non-interacting density–density response function along the imaginary ω axis [12]

$$\chi_0(q, i\omega) = -\nu_0 \left(1 - \frac{\sqrt{2}}{\tilde{q}} \sqrt{a + \sqrt{a^2 + \tilde{\omega}^2}} \right), \tag{10}$$

where $\nu_0 = m/(2\pi\hbar^2)$ is the density of states of a spin-polarized 2D gas, $\tilde{q} = q/k_F$ and $\tilde{\omega} = m\omega/(\hbar k_F^2)$ are the dimensionless wave vector and frequency, respectively, and finally we have defined $a = \tilde{q}^2/4 - \tilde{\omega}^2/\tilde{q}^2 - 1$. Note that the response function along the real ω axis $\chi(q, \omega)$ [12] is used in the pole term (9). With the stated approximations, the excitation spectrum could be written as

$$\varepsilon(k) = \varepsilon_0(k) + \Sigma(k, \varepsilon(k)). \tag{11}$$

In the numerical calculations, we will use the "on-shell approximation", replacing $\varepsilon(k) \to \varepsilon_0(k)$ in the self-energy.

Now we need to approximate the effective dipole–dipole interaction $W(q)$. Within the random-phase approximation, one simply replaces $W(q)$ with the bare interaction $V(q)$. As the Fourier transform of $v_{dd}(r)$ of Eq. (1) requires a short-distance regularization, the final result will depend on this artificial cutoff parameter [22]. A simple resolution to this problem could be achieved through Hubbard local field factor (LFF) [12]. Within the Hubbard approximation the effective dipole–dipole interaction reads

$$\begin{aligned} W_H(q) &= v_{dd}(q) - v_{dd}\left(\sqrt{k_F^2 + q^2}\right) \\ &= \frac{C_{dd}}{2}\left[\sqrt{k_F^2 + q^2} - q\right], \end{aligned} \tag{12}$$

where the expression in the second line is obtained after taking the vanishing cutoff limit. A more elaborate approximation for the effective interaction would be obtained from using fluctuation-dissipation theorem together with the interacting static structure factor $S(q)$ [21]

$$W(q) = \frac{\varepsilon_0(q)}{2n}\left[\frac{1}{S^2(q)} - \frac{1}{S_{HF}^2(q)}\right], \tag{13}$$

where $S_{HF}(q)$ is the non-interacting static structure factor and the interacting static structure factor $S(q)$ could be obtained, e.g., from quantum Monte Carlo simulations [23]. In this work we have used an accurate numerical results for $S(q)$ obtained from the Fermi-Hypernetted-Chain (FHNC) calculations [21].

Finally the many-body effective mass at the Fermi level could be obtained from the slope of interacting excitation spectrum [12]

$$\frac{1}{m^*} = \frac{1}{\hbar^2 k_F} \left.\frac{d\varepsilon(k)}{dk}\right|_{k \to k_F}. \tag{14}$$

3 Numerical Results

Now we turn to the presentation of our numerical results for the self-energy and many-body effective mass. Figures 1 and 2 show different contributions to the single-particle spectrum at two values of the coupling strength λ, calculated within the above mentioned two different approximations (i.e., Hubbard and FHNC) for the effective inter-particle interaction. In both figures, the Fock contribution $u(k)$ to the self-energy has positive slope at the Fermi wave vector and, hence, decreases the effective mass, whereas the dynamic contribution $\Sigma^{(\rho)}(k, \varepsilon_0(k))$ has negative slope and tends to enhance the effective mass. Within the Hubbard approximation, the dynamical contribution dominates over the Fock term at intermediate interaction strengths, while within the FHNC scheme, both contributions to the self-energy are of the same order up to very large coupling constants λ. In both Hubbard and FHNC approximations, one finds a negative slope of the total single-particle spectrum at large λ.

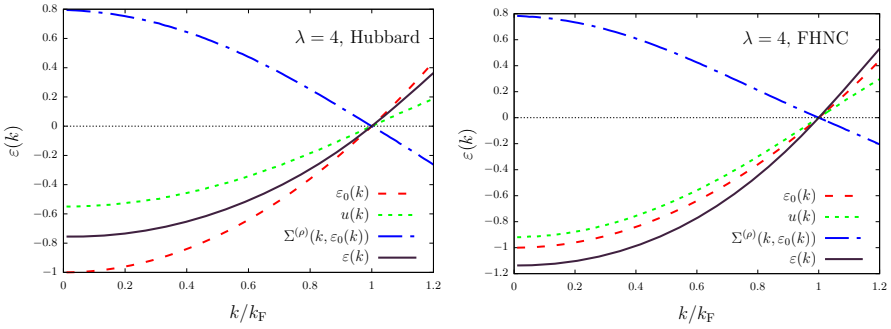


Fig. 1 The single-particle spectrum (in units of $\hbar^2 k_F^2/(2m)$) and different contributions to it, calculated within G_0W approximation at $\lambda = 4$ and within Hubbard (*left*) and FHNC (*right*) approximations to the effective dipole–dipole interaction. Note that all contributions are shifted to become zero at k_F for a better visibility (Color figure online)

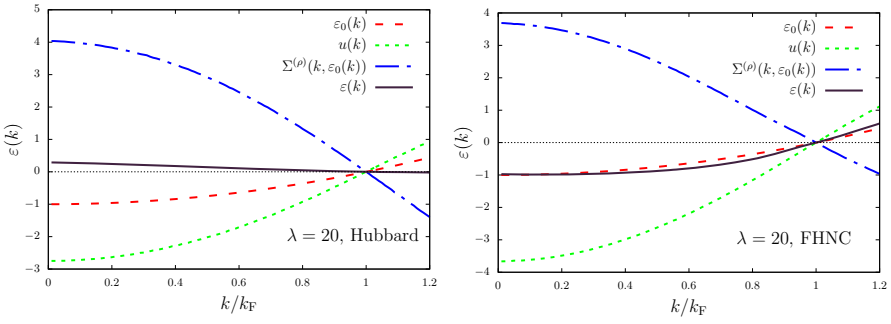


Fig. 2 The single-particle spectrum (in units of $\hbar^2 k_F^2/(2m)$) and different contributions to it, calculated within G_0W approximation at $\lambda = 20$ and within Hubbard (*left*) and FHNC (*right*) approximations to the effective dipole–dipole interaction. Note that all contributions are shifted to become zero at k_F for a better visibility (Color figure online)

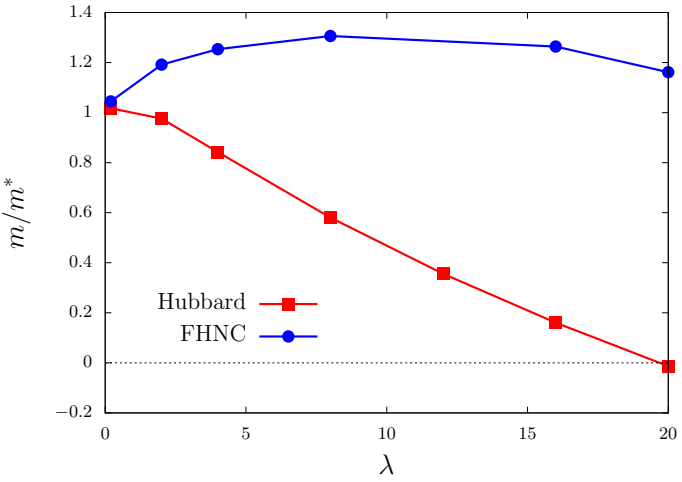


Fig. 3 The relative effective mass of a 2D dipolar Fermi liquid as a function of the dimensionless coupling constant λ, calculated within the G_0W approximation and with Hubbard and FHNC approximations for the effective dipole–dipole interaction (Color figure online)

In Fig. 3 we present our numerical results for the relative effective mass m/m^* within Hubbard and FHNC approximations for the effective interaction. Hubbard approximation results in a strong enhancement of the effective mass. This quantity diverges at $\lambda \approx 20$. A more accurate treatment of the exchange-correlation holes within the FHNC scheme results in a large cancellation between Fock and dynamical contributions to the self-energy and the effective mass does not deviate significantly from its bare value up to $\lambda \approx 20$. Note that at larger coupling strengths the effective mass calculated within the FHNC approximation diverges too (not shown in the figure).

4 Summary and Conclusion

We have calculated the many-body effective mass for a spin-polarized 2D system of fermions interacting via dipole–dipole interaction. We have used the G_0W approximation along with two models of effective dipole–dipole interactions in the system. Our results show that the effective mass is enhanced by interaction effects and diverges at a critical coupling strength. The enhancement is due to the density fluctuations in the system as there are no spin fluctuations. The divergence at large λ is similar to the situation in 2D liquid ^{3}He [19], and further work is needed to discern its physical meaning. It would be interesting to have experimental results for the effective mass of dipolar gases. Time-of-flight measurements on strongly interacting polar molecules or magnetic atoms are naturally expected to shed light on the effects of many-body interactions on effective mass.

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