Density fluctuation spectrum of two-dimensional correlated fermion systems

Akihiro Kotani and Dai Hirashima
Department of Physics, Nagoya University, Nagoya 464-0862, Japan
E-mail: kotani@s.phys.nagoya-u.ac.jp

Abstract. Density fluctuation spectrum of two-dimensional fermions that interact with short-range repulsive interaction is calculated with the self-consistent perturbation theory. The spectrum extends beyond the particle-hole continuum band in the noninteracting case because of the multiparticle excitations. At a large wave vector, a peak develops in the spectrum near the lower threshold of the particle-hole continuum. These results are compared with the recent inelastic neutron scattering experiment on two-dimensional $^3$He adsorbed on graphite.

1. Introduction

Godfrin et al.[1] performed an inelastic neutron scattering experiment on monolayer liquid $^3$He adsorbed on graphite. They were able to observe the particle-hole continuum band (PHB) characterizing the fermi liquid state of two-dimensional liquid $^3$He. At a small wave vector, $q \simeq k_F$, where $k_F$ is the fermi wave vector, they found a peak at a frequency higher than the PHB. They ascribed it to the the zero sound mode (ZSM). The zero sound mode (ZSM) was found to enter the PHB at an intermediate wave vector. At a larger wave vector, $q \simeq 3k_F$, a peak in the spectrum was again found. This time, the peak was found below the PHB. This implied that the ZSM re-appeared below the PHB at large wave vectors. Then, the dispersion relation of the ZSM could be very similar to the phonon-roton dispersion curve in superfluid $^4$He.

The experimental results were analyzed using the random phase approximation (RPA). In the RPA, the threshold of the PHB is unchanged from that in the noninteracting case. To understand the experimental results correctly, we have to consider the correlation effect. In this contribution, we study the correlation effect on the dynamical responses of two-dimensional fermion systems. In particular, we pay attention to the density fluctuation spectrum at large wave vectors and show that the spectrum extends below the threshold of the noninteracting PHB and, at the same time, the peak in the spectrum shifts to a lower energy. Thus, the result is qualitatively consistent with the experimental finding in two-dimensional (2D) $^3$He although no clear mode is present in the large-wave-vector region.

In the small-wave-vector and low-energy region, the Landau fermi liquid theory works and the ZSM is explained with the fermi liquid theory. However, in the large-wave-vector region, the validity of the Landau fermi liquid theory is questionable, and we have to resort to more microscopic approaches. An example is the correlated-basis-function (CBF) theory[2, 3]. Indeed, the CBF theory has been applied to the dynamics of 2D $^3$He and some success has been obtained[4, 5], but it still has room for improving. Another approach is the $T$-matrix
approach[6, 7]. This approach must work well for 2D $^3$He, but has not been fully applied. In this study, we follow a semi-phenomenological approach. We start from an effective short-range interaction potential and explore the effect of the correlation effect on density fluctuation spectrum using perturbation theory with respect to the effective interaction.

2. Model
To facilitate the calculation we consider a dilute fermion system on a square lattice. The number of fermions per lattice point is so small, $n \simeq 0.11$, that the lattice effect is suppressed. In addition to the onsite repulsive interaction, we consider interaction between fermions at different sites. Thus, we study a dilute extended Hubbard model on a square lattice,

$$
H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_n \sum_{(i,j)_n} V^{(n)} n_i n_j,
$$

(1)

where $\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a)$, $n_i = \sum_{\sigma} n_{i\sigma} = \sum_{\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}$, and $(i,j)_n$ stands for the $n$th neighbor pairs. For simplicity, we put $V^{(1)} = V^{(2)} = V_1$ and $V^{(3)} = V^{(4)} = V_2$. At $n \simeq 0.11$, the fermi energy $\epsilon_F$ is given by $\epsilon_F \simeq 0.67t$. In what follows, we study the system at $T = 0.04t \simeq 0.06\epsilon_F$. We choose the values of interaction strength rather arbitrarily. Therefore, the present results are valid only qualitatively.

2.1. RPA
First we study the dynamical density response function $\chi_c(q, \omega)$ with the RPA. Here, we neglect the Fock term in the self-energy, but include the exchange contributions in calculating the density fluctuation spectrum $\text{Im} \chi_c(q, \omega)$. Figure 1 shows $\text{Im} \chi_c(q, \omega)$ at $q = 3k_F$ for $u = U/(4\pi t) = 0.30$ and $v_1 = V_1/(4\pi t) = 0.15$, and $v_2 = 0.06$. It can be seen that the PHB threshold is unchanged from the noninteracting case, but a peak is developed near the lower threshold of the PHB. This result is similar to the experimental one except for the fact that no finite intensity is found below the lower threshold. We note that the spectrum is asymmetric even for $u = 0$. This is because of the lattice effect. For this large-wave-vector region, the lattice effect cannot be completely suppressed. However, the threshold behavior at the lower edge is not significantly affected by the lattice effect.

This RPA result actually suffers from a serious problem. Applying the same approximation to spin fluctuations, we find that the uniform susceptibility diverges for the same parameters. We have to search for parameters where density and spin susceptibilities remain finite or to use a more refined approximation.

![Figure 1](image-url)  
**Figure 1.** Density fluctuation spectrum at $q = 3k_F$ for $u = 0.30$, $v_1 = 0.15$, and $v_2 = 0.06$. Dotted line represents the spectrum in the noninteracting case.
2.2. Selfconsistent second order perturbation theory (SCSOPT)

To avoid the divergence of susceptibility, we go on to the SCSOPT, where, in addition to the Hartree-Fock term, the self-energy terms that are of the second order with respect to interaction (Fig. 2) are selfconsistently calculated. We have found that, in the SCSOPT, finite density and spin susceptibilities are obtained for the parameters used in this study.

Typically, we use the lattice whose size is $L \times L = 2^7 \times 2^7$. We have checked that the finite size effect is negligible. The number of Matsubara frequencies used in the calculations is $2^{10}$. Data on the imaginary axis are analytically continued to the real axis using the Padé approximation.

When we calculate the density fluctuation spectrum, we have to consider the vertex corrections corresponding to the second-order self-energy shown in Fig. 2. The irreducible vertex corrections can be uniquely determined so that the Ward identities are satisfied. To obtain the full vertex corrections, we have to solve integral equations, which is a formidable task in general. However, if we can use the fast Fourier transformation (FFT), we can efficiently solve the integral equations. In the absence of $V_i$, the integral equations are of a convolution form and can be solved with the FFT. In the presence of finite $V_i$, however, the FFT cannot be applied. We thus make approximations for the integral equations for the full vertex corrections. The approximations are essentially (partially) local approximations. The details will be reported elsewhere.

To check the validity of the approximations, we compare the compressibility $\chi_c = \partial n/\partial \mu$, where $\mu$ is the chemical potential, calculated from the single-particle Green’s function and $\chi_c(q \to 0, \omega = 0)$ calculated from the density fluctuation spectrum. This is equivalent to checking the identity (the compressibility sum rule)

$$\chi_c = 2 \int_{-\infty}^{\infty} \frac{d\omega}{\omega} C(q \to 0, \omega),$$  \hspace{1cm} (2)

where $C(q, \omega) = \text{Im} \chi_c(q, \omega)/[\pi(1 - e^{-\beta\omega})]$. Figure 3 shows the comparison of both sides of Eq. (2) as a functions of $u(= 2.0v_1 = 5.0v_2)$. We can see that the compressibility sum rule is satisfied accurately.

Figure 4 shows the density fluctuation spectrum at $q = 3k_F$ for $u = 0.30$ and $0.50; v_1 = 0.5u$ and $v_2 = 0.2u$ in both cases. It can be seen that the peak in the spectrum shifts to a lower
energy with increasing $u$ as in the case with the RPA. In contrast to the RPA result, the spectrum extends beyond the noninteracting PHB threshold and remains finite down to $\omega = 0$. This is because of the effect of the self-energy correction, in other words, the effect of the multiparticle excitations. In particular, for $u = 0.50$, significant intensity is found below the noninteracting PHB threshold.

![Figure 4. Comparison of the lhs (solid dots) and rhs of Eq. (2) (open squares) for $u : v_1 : v_2 = 1.0 : 0.5 : 0.2$.](image)

### 3. Discussion

We have studied the dynamical density correlation function of 2D fermion systems taking account of the correlation effect. In the small-wave-vector region, we find the ZSM peak develop in the spectrum (although the result is not shown in this paper). In the large-wave-vector region, the peak in the density fluctuation spectrum is found to shift to a lower energy. At the same time, the spectrum is found to extend beyond the PHB threshold in the noninteracting case. Although we did not find a peak below the noninteracting PHB threshold at $q = 3k_F$, our result implies that, at a large wave vector, a peak can develop near (or below) the PHB threshold in the density fluctuation spectrum of correlated fermion systems, although it is not a very well defined ZSM mode. More direct comparison with the experiment on $^3$He is possible only after a realistic calculation using actual interatomic interaction potential is carried out.

In this paper, we have concentrated on the density fluctuations. Neutron scattering can also probe spin fluctuations. A preliminary calculation shows that the intensity of spin fluctuation spectrum is comparable in magnitude with that of density fluctuation spectrum at $q = 3k_F$. If the ratio of the incoherent scattering to the coherent one is small (as in the case of 3D $^3$He[8]), the contribution from spin fluctuations is insignificant at a large wave vector. However, spin fluctuations can make a dominant contribution at small wave vectors and has to be considered in explaining the experimental result.

### References

[1] Godfrin H, Meschke M, Lauter M J, Böhm H M, Krotscheck E, and Panholzer M, 2010 J. Low Temp. Phys. 158 147
[2] Krotscheck E, 1982 Phys. Rev. A 26 3536
[3] Böhm H M, Holler R, Krotscheck E and Panholzer M, 2010, Phys. Rev. B 82, 224505
[4] Panholzer M, Böhm H M, Holler R and Krotscheck E, 2010 J. Low Temp. Phys. 158 135
[5] Böhm H M, Krotscheck E, Panholzer M, Godfrin H, Lauter H J and Meschke M, 2010 J. Low Temp. Phys. 158 194
[6] Glyde H R and Hernandi S I, 1984, Phys. Rev. B 29 3873
[7] Glyde H R and Hernandi S I, 1984, Phys. Rev. B 29 4926
[8] Sköld K, Pelizzari C A, Kleb R and Ostrowski G E, 1976, Phys. Rev. Lett. 37 842