Multi-particle-hole excitations in many-body Fermi systems

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Abstract

We formulate a microscopic theory for calculating the dynamic structure function of ^{3}He and other strongly interacting Fermi liquids. The theory is a generalization of the correlated basis function theory for the dynamics of ^{4}He and includes time–dependent *two–particle–two–hole* excitations. It may also be interpreted as a systematic extension of the random–phase approximation (RPA). Comparison of numerical results with experiments show a significant improvement of the excitation spectrum over RPA predictions while maintaining the accuracy of prediction of ground–sate quantities like the static structure function.

Key words: Excitations ; Helium-3 ; dynamic structure factor ; Fermion systems

1. INTRODUCTION

The excitation spectrum of liquid ^{4}He can be quite well understood by generalizing the original Feynman–theory[1] to include time–dependent pair correlations. This is plausible because, in the vicinity of the roton minimum, the wavelength of the excitation is comparable to that of the interparticle distance and, hence, long–wavelength approximations like the randon phase approximation are inapplicable.

The first microscopic calculation of the excitation spectrum of ^{4}He usind fluctuating pair correlations were carried out by Jackson[2] and by Chang and Campbell[3]; later improvements of the implementation of the theory lead to almost perfect agreement between theory and experiment well beyond the roton wave number.[4]

We report here the first implementation of the same ideas for Fermi systems. We assume a *correlated* ground state $\Psi_0(1,\ldots,N) = F(1,\ldots,N)\Phi_0(1,\ldots,N)$, where $\Phi_0(1,\ldots,N)$ is a model wave function, and $F(1,\ldots,N)$ *correlation operator* which is normally taken to be an optimized Feenberg function, alternatively we may assume that $\Psi_0(1,\ldots,N)$ is the exact ground state.

The time–dependent Fermion wave function is taken to be a generalization of the time–dependent Hartree–Fock wave function which includes time–dependent two–particle amplitudes:

$$|\Psi(t)\rangle = \frac{F\,|\Phi(t)\rangle}{\langle\Phi(t)|\,F^\dagger\,F\,|\Phi(t)\rangle^{1/2}}\ ,$$

$$|\Phi(t)\rangle = \mathrm{e}^{-iH_{\mathbf{oo}}\,t/\hbar}\ e^{\frac{1}{2}\,U(t)}\,|\Phi_0\rangle\ , \tag{1}$$

$$U(t) = \sum_{ph}\ c_{ph}(t)\ a_p^\dagger a_h + \frac{1}{2}\sum_{pp'hh'}\ d_{pp',hh'}(t)\ a_p^\dagger a_{p'}^\dagger a_{h'} a_h\ . \tag{2}$$

In analogy to defining the model ground state by a variational principle, we determine the *perturbed* system by a stationarity principle. The action integral is defined by

$$S\left[c_{ph}, c_{ph}^*, d_{pp'hh'}, d_{pp'hh'}^*\right] = \int dt\ L(t)\ , \tag{3}$$

where the Lagrangian has the form

$$L(t) = \left\langle \Psi(t)\,\middle|\, H + h_{\mathrm{ext}}(\mathbf{r};t) - i\,\hbar\frac{\partial}{\partial t}\,\middle|\,\Psi(t)\right\rangle\ , \tag{4}$$

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q [Å^{-1}]	ω_1 [K]	ω_2 [K]	CRPA	2p-2h
0.3	1.15	5.8	6.0	3.7
0.4	1.15	7.5	8.1	6.0
0.5	1.15	8.7	11.0	8.0
0.6	1.15	10.5	13.5	10.0
0.7	1.15	12.1	16.0	12.5
0.8	1.15	12.8	18.5	14.5

Table 1
Experimental data from neutron scattering experiments of Glyde *et. al.*[6]. The energies ω_i are the location of the peaks in the data at a temperature of 0.1 K. The peak at low energies is the spin-fluctuation scattering and at higher energies it secribes the the zero sound mode. In the last two columns are the energies of the peak in the correlated RPA and for our 2p-2h calculation.

where $h_{\rm ext}(\mathbf{r};t)$ describes a small, external perturbation. The action integral is made stationary under variations of the $c_{ph}(t)$ and $d_{pp',hh'}(t)$, omitting the $d_{pp',hh'}(t)$ leads to the (correlated)RPA.

The equations of motion are significantly more complicated than the RPA, but they can be manipulated, employing approximations that lead to the boson result in the appropriate limit, to give a closed–form expression for the dynamic structure function. Central to the derivation is a *local approximation* which assumes that the 2p–2h amplitudes $d_{pp',hh'}(t)$ are matrix elements of a local operator $d(\mathbf{r},\mathbf{r}';t)$. The resulting form of the dynamic structure function is then[5]:

$$\chi^{(\mathrm{2p2h})}(q,\omega) = 2\left[\chi_0(q,\omega) + \frac{S(q)}{S_F(q)}\,\chi_0^{(-)}(q,\omega)\,\chi_0^{(+)}(q,\omega)\,\left(\tilde{V}_{xx}+\tilde{V}_{yy}-\tilde{V}_{xy}-\tilde{V}_{yx}\right)\right]\Big/$$
$$\Big/\left[2+\chi_0^{(-)}\,\left(\tilde{V}_{xx}+\tilde{V}_{xy}\right)-\chi_0^{(+)}\left(\tilde{V}_{yy}+\tilde{V}_{yx}\right)-\right. \qquad (5)$$
$$\left.-\frac{S(q)}{S_F(q)}\,\left[\chi_0^{(+)}(\tilde{V}_{yy}-\tilde{V}_{yx})+\chi_0^{(-)}(\tilde{V}_{xy}-\tilde{V}_{xx})-2\,\chi_0^{(+)}\chi_0^{(-)}(\tilde{V}_{xx}\tilde{V}_{yy}-\tilde{V}_{xy}\tilde{V}_{yx})\right]\right]\,.$$

where the V_{ij} are different local channel interactions, and

$$\chi_0^{(\pm)}(q,\omega) = \frac{1}{N}\sum_h \frac{n(h)\,(1-n(h+q))}{\hbar\omega \mp e_{h+q\,h} \pm i\eta}\,, \qquad (6)$$

are channel Lindhard functions.

2. APPLICATIONS

Table 1 compares the peak location of our calculated dynamic structure function with that of the correlated RPA and with the experiments of Ref. [6]. Note that we are, here, not concerned with spin fluctuations, therefore we do not reproduce the spin–fluctuation peak. Otherwise, it is evident that including time–dependent pair correlations leads to a significant improvement of the theoretical predictions over the RPA.

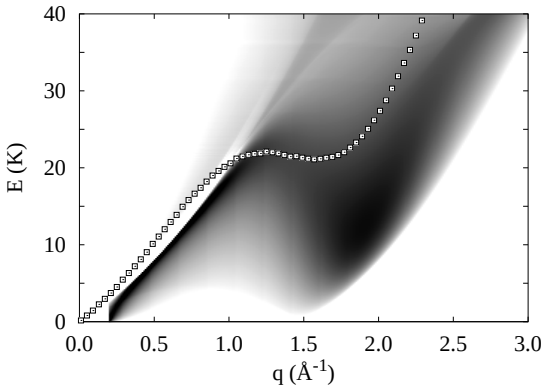

Fig. 1. Dynamic structure function for the calculation including time–dependent pair correlations. The boxes represent the Feynman excitation spectrum $\hbar^2q^2/2mS(q)$. The grey scale ranges from white for zero to black for the highest absorption.

More details on the dynamic structure function are shown in figure 1.

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