Quantitative comparison between theoretical predictions and experimental results for Bragg spectroscopy of a strongly interacting Fermi superfluid

Peng Zou\(^1\), Eva D. Kuhnle\(^2\), Chris J. Vale\(^2\), and Hui Hu\(^2\)

\(^1\)Department of Physics, Renmin University of China, Beijing 100872, China and
\(^2\)ARC Centre of Excellence for Quantum-Atom Optics and Centre for Atom Optics and Ultrafast Spectroscopy, Swinburne University of Technology, Melbourne 3122, Australia

(Dated: January 6, 2011)

Theoretical predictions for the dynamic structure factor of a harmonically trapped Fermi superfluid near the BEC-BCS crossover are compared with recent Bragg spectroscopy measurements at large transferred momenta. The calculations are based on a random-phase (or time-dependent Hartree-Fock-Gorkov) approximation generalized to the strongly interacting regime. Excellent agreement with experimental spectra at low temperatures is obtained, with no free parameters. Theoretical predictions for zero-temperature static structure factor are also found to agree well with the experimental results and independent theoretical calculations based on the exact Tan relations. The temperature dependence of the structure factors at unitarity is predicted.

PACS numbers: 05.30.Fk, 03.75.Hh, 03.75.Ss, 67.85.-d

Ultracold Fermi gases of \(^6\)Li and \(^40\)K atoms near Feshbach resonances provide a new paradigm for studying strongly correlated many-body systems [1]. At low temperatures, they display the intriguing crossover from a Bose-Einstein condensate (BEC) to a Bardeen-Cooper-Schrieffer (BCS) superfluid \(^2\). In the unitarity regime at the cusp of the crossover, a superfluid with neither dominant bosonic nor fermionic character emerges that exhibits universal properties that might be found in other strongly interacting superfluids \(^2\) \(^3\), such as high-temperature superconductors or nuclear matter in neutron stars. This new superfluid has already been investigated intensively \(^1\) \(^2\), leading to several milestone observations, some of which still defy theoretical understanding. Here we present a quantitative description of the recent two-photon Bragg spectroscopy measurement for this new superfluid \(^3\).

Theoretical challenges in describing the BEC-BCS crossover arise from its strongly correlated nature: there is no small interaction parameter to set the accuracy of theories \(^9\). Significant progress has been made in developing better quantum Monte Carlo simulations \(^7\) \(^10\) and strong-coupling theories \(^2\) \(^11\) \(^14\), leading to the quantitative establishment of a number of properties. These include equation of state \(^6\) \(^7\) \(^12\) \(^13\) \(^17\), frequency of collective oscillations \(^18\) \(^19\), pairing gap \(^10\) \(^20\), and superfluid transition temperature \(^8\) \(^21\). However, other fundamental properties, such as the single-particle spectral function measured by rf spectroscopy \(^22\) \(^23\) and the dynamic structure factor probed by Bragg spectroscopy \(^5\), are not as well understood.

In this Rapid Communication, we show that a random-phase approximation (RPA), generalized to the strongly interacting regime, is able to describe quantitatively the observed Bragg spectra for harmonically trapped \(^6\)Li atoms at large transferred momenta. This surprising result indicates that the RPA captures the essential physics and constitutes a reasonable approximation for the strongly interacting region of the BEC-BCS crossover, particularly the low temperature range accessed by most experiments. The RPA method has previously been used to study the dynamic structure factor \(^24\) and collective oscillations \(^25\) of weakly interacting Fermi superfluids. A dynamic mean-field approach, identical to the RPA but based on kinetic equations, was developed to investigate structure factors \(^20\) and collective modes \(^27\) of a uniform, strongly interacting Fermi gas. At finite temperatures, structure factors at the crossover were also studied using a pseudogap theory \(^28\).

Our main result is summarized in Fig. 1, which shows the normalized experimental Bragg spectra \(^5\) along with the RPA predictions. Excellent agreement is found, with
no free parameters.

We begin by outlining briefly the RPA using the Hamiltonian (hereafter \( h = 1 \)),

\[
\mathcal{H} = \sum_{\sigma} \int d^3r \left[ \frac{\nabla^2}{2M} - \mu + V_T(r) \right] \psi_{\sigma}(r) + U_0 \int d^3r \psi^+_{\alpha}(r) \psi^+_{\beta}(r) \psi_{\beta}(r),
\]

which describes a balanced spin-1/2 (\( \sigma = \uparrow, \downarrow \)) Fermi gas with mass \( M \) in a harmonic trap \( V_T(r) \), where fermions with unlike spins interact via a contact potential \( U_0 \delta(\mathbf{r} - \mathbf{r}') \). The total number of atoms \( N \) is tuned by the chemical potential \( \mu \) and the bare interaction strength \( U_0 \) is renormalized by the s-wave scattering length \( a \), \( 1/U_0 + \sum_{k} M/k^2 = M/(4\pi a) \). In the superfluid phase, we treat the system as a gas of long-lived Bogoliubov quasiparticles interacting through a mean-field and consider its response to a weak external field of the form \( \delta V e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} \). The essential idea of the RPA is that there is a self-generated mean-field potential experienced by quasiparticles \( \tilde{\mathcal{U}} \), associated with the local changes in the density distribution of the two spin species, \( \delta \mathcal{U} = U_0 \int d^3r \sum_{\sigma} \delta n^{+}_{\sigma}(r,t) \psi_{\sigma}^+ \psi_{\sigma}(r,t) + \delta m^{+}(r,t) \psi_{\sigma}^+ \psi_{\sigma}(r,t) + m^{+}\psi_{\sigma} \psi_{\sigma}(r,t) \), where \( \delta n_{\sigma} \equiv \delta n_{\sigma}(r,t) \) and \( \delta m \equiv \delta m(r,t) \) are the normal and anomalous density fluctuations, respectively, which must be determined self-consistently. In the linear approximation, the self-generated potential \( \delta \mathcal{U} \) plays the same role as the perturbation field when we calculate the dynamic response using a static BCS Hamiltonian as the reference system \( \tilde{\mathcal{U}} \). This leads to coupled equations for density fluctuations. The linear response is characterized by a matrix consisting of all two-particle response functions:

\[
\chi \equiv \left\{ \begin{array}{c} \langle \hat{n}_{\uparrow}(\mathbf{r}) \hat{n}_{\downarrow}(\mathbf{r}) \rangle \\ \langle \hat{n}_{\uparrow}(\mathbf{r}) \hat{n}_{\uparrow}(\mathbf{r}) \rangle \\ \langle \hat{n}_{\downarrow}(\mathbf{r}) \hat{n}_{\uparrow}(\mathbf{r}) \rangle \\ \langle \hat{n}_{\downarrow}(\mathbf{r}) \hat{n}_{\downarrow}(\mathbf{r}) \rangle \\ \langle \hat{m}_{\uparrow}^+ \hat{m}_{\downarrow}^+ \rangle \\ \langle \hat{m}_{\downarrow}^+ \hat{m}_{\uparrow}^+ \rangle \\ \langle \hat{m}_{\uparrow}^+ \hat{m}_{\uparrow}^+ \rangle \\ \langle \hat{m}_{\downarrow}^+ \hat{m}_{\downarrow}^+ \rangle \end{array} \right\},
\]

where \( \langle \hat{A}\hat{B} \rangle \) is the Fourier transform of the retarded function \(-i\theta(t - t')\). For simplicity, we abbreviate \( \chi_{\sigma\sigma} \equiv \langle \hat{n}_{\sigma}\hat{n}_{\sigma} \rangle \), \( \chi_{\sigma m} \equiv \langle \hat{n}_{\sigma}\hat{m}_{\sigma} \rangle \), \( \chi_{\sigma m} \equiv \langle \hat{m}_{\sigma}\hat{n}_{\sigma} \rangle \), and so on. By solving the coupled equations for density fluctuations, the standard RPA response function \( \chi \) can be expressed in terms of the static BCS response function \( \chi^0 \) and the static structure factor \( S_{\sigma\sigma'}(\omega) \) is given by:

\[
\chi = \chi^0 \left[ 1 - U_0 \chi^0 G \right]^{-1},
\]

where \( G = \delta(\mathbf{r} - \mathbf{r}')[\sigma_0 \otimes \sigma_\sigma] \) is a direct product of two Pauli matrices \( \sigma_0 \) and \( \sigma_\sigma \) and the unit matrix \( I = \delta(\mathbf{r} - \mathbf{r}')[\sigma_0 \otimes \sigma_0] \). The dynamic structure factor \( S_{\sigma\sigma'}(\omega) \) is related to the normal density response function by the fluctuation-dissipation theorem:

\[
S_{\sigma\sigma'}(\omega) = -\frac{1}{\pi} \frac{1}{[1 - \exp(-\omega/k_B T)]} \text{Im} \chi_{\sigma\sigma'}(\omega),
\]

and the UV divergence is canceled exactly by the small value of \( U_0 \), when the momentum cut-off goes to infinity. In homogeneous systems, a careful account of the divergent terms in the inverted matrix of the RPA equation (2) leads to a concise expression for the response functions:

\[
\chi^{\uparrow\downarrow} = \chi^{\uparrow\downarrow} - \chi^{\uparrow\uparrow} + \chi^{\downarrow\downarrow},
\]

where the response functions with a tilde, i.e., \( \tilde{\chi}_{m\bar{m}} \equiv \chi_{m\bar{m}} + \sum_{k} M/k^2 - M/(4\pi a) \), become free from any ultraviolet divergence. The above equations were previously obtained by Combes and collaborators using kinetic equations (see Eq. (22) in Ref. 27). Note that, we use a Leggett-BCS ground state without inclusion of the Hartree-Fock term in the quasiparticle spectrum. Therefore, in the BCS regime our treatment does not account for the leading interaction effect as in Refs. 24, 25. At the crossover, however, it does capture the dominant pairing gap. Note also that, the RPA method accounts for single particle-hole excitations. Higher correlations such as multi-particle-hole excitations are neglected.

In the presence of a harmonic trap, the renormalization procedure becomes cumbersome because of the discrete energy levels. It is convenient to use a local density approximation (LDA) that treats the system as a collection of many homogeneous cells with local chemical potential \( \mu(r) = \mu - V_T(r) \), where \( V_T(r) = M(\omega^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2 \) is the harmonic trapping potential. The LDA treatment is valid for a large number of atoms such as \( N \sim 10^5 \) as in experiments. It has been used extensively in studying the static density profile of either atomic Fermi, Bose gases or Bose-Fermi mixtures. In the nuclear context, it has also been used to calculate the dynamic response function \( \chi^0 \). At a given temperature and scattering length, we solve the Leggett-BCS equation with local chemical potential for the local pairing gap and calculate the static response function \( \chi^0 \), then solve the local RPA density response functions using Eqs. (4) and (5), and finally obtain the total RPA responses by integrating over the whole trap.
In our calculations, the interaction strength is characterized by the dimensionless parameter, $1/(k_F a)$, where $k_F = \sqrt{2M E_F}$ is the Fermi wave vector and the Fermi energy is $E_F = (3N\omega_x\omega_y\omega_z)^{1/3}$.

RPA predictions agree well with the experimental results in the unitarity regime ($1/k_F a = 0.0$ and $0.2$) and BEC regime ($1/k_F a = 0.8$). The agreement on the BCS side ($1/k_F a = -0.5$), however, becomes worse. The quantitative agreement around unitarity is very compelling, since the RPA was assumed to be unreliable in the (strongly interacting) regime of large pair fluctuations. Our comparison indicates that the RPA is able to describe the dynamical properties of the BEC-BCS crossover, at least at zero temperature and large momenta. High order multi-particle-hole excitations, absent in the RPA theory, seems to be negligibly small at large momenta. More studies are needed to understand this. Note finally that, the somewhat poorer agreement at $1/k_F a = -0.5$ can be attributed to the mean-field shift, which is ignored in the RPA but dominates for sufficiently weak interactions.

Figure 2: (color online). Zero temperature spin parallel $S_{\uparrow\uparrow}(q,\omega)$ (dashed lines), anti-parallel $S_{\uparrow\downarrow}(q,\omega)$ (dot-dashed lines), and total dynamic structure factor $S(q,\omega) = 2[S_{\uparrow\uparrow} + S_{\uparrow\downarrow}]$ (solid lines) across the BEC-BCS crossover: $1/k_F a = 0.5$ (a), $0.0$ (b), and $-0.5$ (c). The negative weight in $S_{\uparrow\downarrow}$ at about the recoil energy is consistent with the exact sum rule $\int \omega S_{\uparrow\downarrow}(q,\omega) d\omega = 0$ [36].

Figure 3: (color online). Quantitative comparison between theory and experiment for the zero temperature static structure factor across the crossover. For $S_{\uparrow\downarrow}$, with no free parameters our RPA prediction (plus symbols) agrees well with the experimental data for $S(q,\omega) - 1$ (solid circles with error bars) [35] and an independent theoretical result based on the exact Tan relations (solid line) [36]. At large transferred momentum, $S_{\uparrow\uparrow} \simeq 1$. The inset highlights the RPA prediction with respect to the Tan-relation result in the BEC regime.

The agreement between the RPA theory and the Bragg experiment is further confirmed by comparing the spin anti-parallel static structure factor at zero temperature, as reported in Fig. 3. Experimentally, the static structure factor can be measured model-independently by invoking the $f$-sum rule [35]; while, theoretically, it can be determined very accurately using the exact Tan relations and the known equation of state [36]. It is evident from Fig. 3 that the RPA prediction fits very well with the experimental data, as well as the independent theoretical result based on the Tan relations. In particular, the two theoretical predictions are nearly indistinguishable on the BEC side with $1/k_F a \geq 0$. However, they differ towards the BCS limit, as highlighted in the inset. The discrepancy is consistent with Fig. 1d where the RPA predicts less pairing and hence lower $S(q)$.
interacting Fermi gas at finite temperatures and low momenta.

We are indebted to P. Drummond, P. Hannaford, W. Zhang and N.-H. Tong for fruitful discussions. Numerical calculations were performed at the Physics Laboratory for High Performance Computing, Renmin University of China. This work was supported by the ARC Centre of Excellence for Quantum-Atom Optics, ARC Discovery Project Nos. DP0984522 and DP0984637, and NSFC Grant No. 10774190. Correspondence should be addressed to IH at lhu@swin.edu.au.

Figure 4: (color online). Temperature dependence of the dynamic (a) and static (b) structure factor for a unitary Fermi gas in harmonic traps at \( q = 5k_F \). According to the Tan relation, \( S_{11}(q) \simeq 128\xi/[175\xi^{1/4}(q/k_F)] \) at \( T = 0 \) \[32\], where \( \xi \) and \( \zeta \) are the universal parameters at unitarity \[17\]. The symbols in (b) show predictions using theoretically or experimentally determined \( \xi \) and \( \zeta \): ENS experiment (square) \[17\], Gaussian pair fluctuation theory (circle) \[12\], and self-consistent theory (triangle) \[57\]. Here, \( T_c \simeq 0.377T_F = 0.37E_F/k_B \).

A more stringent test of the RPA theory may be provided by the temperature or momentum dependence of dynamic and static structure factors. In Fig. 4, we predict the dynamic and static structure factor as a function of temperature for a trapped Fermi gas at unitarity, which will be investigated in future experiments. As anticipated, the pair (atomic) response increases (decreases) with decreasing the temperature, leading to a monotonic decay of the static structure factor.

The present RPA theory is most likely valid only in a narrow temperature window near \( T = 0 \). With increasing temperature, the pairing gap decreases and thermal pair fluctuations increase. The RPA will eventually break down at a characteristic temperature \( T_{RAPA} \lesssim T_c \). This is evident in Fig. 4b where the spin anti-parallel static structure factor vanishes unphysically above the superfluid transition temperature.

At low transferred momenta, quantum fluctuations are likely to increase and the RPA theory will become less reliable. To overcome these limitations, we could use a Cooperon-mediated interaction (many-body \( T \)-matrix) to replace the bare contact interaction \[38\], or use the phenomenological Landau parameters for the mean-field shift \[39\], as determined from thermodynamic measurements \[10\], or quantum Monte Carlo simulations.

In summary, we have used a strong-coupling RPA theory to calculate the dynamic and static structure factors of a trapped Fermi gas at the BEC-BCS crossover. The theory is quantitatively applicable at low temperatures and large transferred momenta, as confirmed by the excellent agreement with the experimental Bragg spectra. The RPA theory thus seems to provide a novel starting point for investigating dynamic properties of a strongly interacting Fermi gas.

[1] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
[2] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 80, 1215 (2008).
[3] T.-L. Ho, Phys. Rev. Lett. 92, 090402 (2004).
[4] H. Hu, P. D. Drummond, and X.-J. Liu, Nature Phys. 3, 469 (2007).
[5] G. Vevavalli et al., Phys. Rev. Lett 101, 250403 (2008).
[6] H. Hu, X.-J. Liu, and P. D. Drummond, New J. Phys. 12, 063038 (2010).
[7] G. E. Astrakharchik et al., Phys. Rev. Lett. 93, 200404 (2004).
[8] A. Bulgac, J. E. Drut, and P. Magierski, Phys. Rev. Lett. 96, 090404 (2006).
[9] E. Burovski et al., Phys. Rev. Lett. 101, 090402 (2008).
[10] J. Carlson and S. Reddy, Phys. Rev. Lett. 100, 150403 (2008).
[11] Y. Ohashi and A. Griffin, Phys. Rev. Lett. 89, 130402 (2002); Phys. Rev. A 67, 063612 (2003).
[12] H. Hu, X.-J. Liu, and P. D. Drummond, Europhys. Lett. 74, 574 (2006).
[13] X.-J. Liu and H. Hu, Phys. Rev. A 72, 063613 (2005).
[14] R. Haussmann et al., Phys. Rev. A 75, 023610 (2007).
[15] L. Luo et al., Phys. Rev. Lett. 98, 080402 (2007).
[16] S. Nasimbene et al., Nature 463, 1057 (2010).
[17] N. Navon et al., Science 328, 729 (2010).
[18] H. Hu et al., Phys. Rev. Lett. 93, 190403 (2004).
[19] A. Altmeyer et al., Phys. Rev. Lett. 98, 040401 (2007).
[20] C. H. Schunck et al., Science 316, 867 (2007).
[21] M. Horikoshi et al., Science 327, 442 (2010).
[22] J. P. Gaebler et al., Nature Phys. 6, 569 (2010).
[23] H. Hu et al., Phys. Rev. Lett. 104, 240407 (2010).
[24] A. Minguzzi, G. Ferrari, and Y. Castin, Eur. Phys. J. D 17, 49 (2001).
[25] G. M. Bruun and B. R. Mottelson, Phys. Rev. Lett 87, 270403 (2001).
[26] R. Combescot, S. Giorgini, and S. Stringari, Europhys. Lett. 75, 695 (2006).
[27] R. Combescot, M. Yu. Kagan, and S. Stringari, Phys. Rev. A 74, 042717 (2006).
[28] H. Guo, C.-C. Chien, and K. Levin, Phys. Rev. Lett. 105, 120401 (2010).
[29] X.-J. Liu et al., Phys. Rev. A 69,043605 (2004).
[30] P. Pieri and G. C. Strinati, Phys. Rev. B 61, 15370 (2000).
[31] X.-J. Liu, H. Hu, and P. D. Drummond, Phys. Rev. A 75, 023614 (2007).
[32] X.-J. Liu, M. Modugno, and H. Hu, Phys. Rev. A 68, 053605 (2003).
[33] P. Schuck et al., Progr. Part. Nucl. Phys. 22, 181 (1989).
[34] A. Brunello et al., Phys. Rev. A 64, 063614 (2001).
[35] E. D. Kühnle et al., Phys. Rev. Lett. 105, 070402 (2010).
[36] H. Hu, X.-J. Liu, and P. D. Drummond, Europhys. Lett. 91, 20005 (2010).
[37] R. Haussmann, M. Punk, and W. Zwerger, Phys. Rev. A 80, 063612 (2009).
[38] H. P. Büchler, P. Zoller, and W. Zwerger, Phys. Rev. Lett. 93, 080401 (2004).
[39] S. Stringari, Phys. Rev. Lett. 102, 110406 (2009).