LA-UR-97- 580

CONF-961258--2

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SUBMITTED TO: Proceedings of Condensed Matter Theories XX Workshop, Pune, India, December 1996, To be published by World Scientific

Los Alamos

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FORM NO. 836 R4
ST. NO. 2629 5/81

BOSE CONDENSATION IN ^{4}He AND NEUTRON SCATTERING

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The discovery of superfluidity in liquid ^4He below $T_\lambda = 2.17^o K$, and its phenomenological characterization since then, has been one of the great success stories of condensed matter physics. The relation of superfluidity to the behavior of atoms was conjectured by F. London in 1938. Superfluidity is a manifestation of the Bose condensation of helium atoms, the extensive occupation of the zero momentum state. Ever since ^4He has been the paradigm in the search for Bose condensates in other systems. At the Pune meeting we have heard exciting new evidence for Bose condensates of laser cooled alkali atoms in magnetic traps [1], of excitons in Cu_2O [2], and possibly pre-formed Cooper pairs of electrons in the high T_c perovskite superconductors [3]. There remains the holy-grail of forming a Bose condensate in spin-polarized hydrogen [4].

Laser cooled alkali atoms in magnetic traps [1] are much closer to ideal Bose condensation than superfluid ^4He. The densities are low, interaction effects are small, and they can be approximated as a weakly interacting dilute Bose gas. The fraction of atoms n_o condensed in the zero momentum state proceeds from zero at a critical temperature $T = T_c$ to nearly one at $T = 0^o K$. The momentum distribution $n(p)$ has a δ-function spike at $p = 0$ with an integrated intensity of n_o. The momentum distribution can be measured by experiments in which the magnetic trap is released, allowing the velocities of the escaping atoms to be observed by time-of-flight. The results conform to expectations within small corrections. Very recent experiments have discovered quantum coherent phenomena such as the atomic equivalent of lasing and quantum interference between two traps.

In contrast, liquid ^4He is a strongly interacting Bose system. That complicates the experimental verification of F. London's prediction that the superfluid transition should be associated with an $n_o\delta(p)$ spike in $n(p)$. The strong interactions dramatically alter $n(p)$ from an ideal Bose gas. Sophisticated many-body calculational methods, such as Greens Function Monte Carlo [8] (GFMC) for zero temperature and

Path Integral Monte Carlo [9] (PIMC) methods for non-zero temperatures, have been developed for such problems. They predict an n_o of only about 0.10 at $T = 0^o K$. This small value contrasts with alkali Bose condensates where n_o is near one. The 90% non-condensate ^4He atoms undergo quantum zero-point motion with momenta spread over a width of about $1\mathring{A}^{-1}$.

In the current excitement for new types of Bose condensates, and new phenomena such as atom lasers, it may be useful to recall the older story of the experimental verification of a relation between superfluidity and Bose condensation in ^4He. This topic has been investigated over many years by neutron scattering experiments and quantum many-body theory. My goal is to illustrate the difficulties of establishing the existence of a Bose condensate in a strongly interacting system, even though its macroscopic effects are manifest. I assume readers have access to a review by Silver and Sokol [5] which emphasizes the neutron scattering theory through 1990 and a review by Snow and Sokol [6] of the *deep inelastic neutron scattering* (DINS) (or *neutron Compton scattering*) experiments through 1995. Another good source is the 1989 book *Momentum Distributions* which addresses related Compton scattering experiments throughout physics. These reviews present the details, equations and data. I focus here on the key concepts, the current status and some recent developments. The insight gained may also be useful for other momentum distribution studies.

Direct experimental observation of $n(p)$ in ^4He has proved elusive. It can not be measured by kinetic experiments on escaping atoms, because ^4He is self bound. Hohenberg and Platzman [10] suggested in 1966 that the best hope for measuring $n(p)$ is DINS. This is the neutron analogue of X-ray Compton scattering measurements of electron momentum distributions in solids and molecules. But after decades of effort and hundreds of research papers, the conclusion reached is that the strong interactions among ^4He atoms invalidate a simple *impulse approximation* (IA) interpretation of DINS experiments. The Bose condensate δ-function predicted in the dynamical structure function by the IA is irretrievably broadened. Only circumstantial evidence remains for a correlation between superfluidity and Bose condensation in ^4He. It consists of excellent quantitative agreement between experiment and *ab-initio* many-body theories, which predict a Bose condensate. But this requires a more sophisticated theory for what DINS measures than the IA.

More generically, *deep inelastic scattering* refers to experiments in which a high energy probe particle scatters at sufficient energy $\hbar\omega$ and momentum $\hbar Q$ transfers that the incoherent dynamical structure function for single particle scattering dominates the coherent structure function for interference scattering between particles. For this concept to be applicable to neutron scattering from ^4He, Q and ω must be much larger than the scales set by the phonon-roton spectrum or the static structure function, $S(Q)$, related by Fourier transform to the radial distribution function $g(r)$. This scale is approximately $Q \geq 5\mathring{A}^{-1}$. The *impulse approximation* (IA) to deep inelastic scattering further assumes that a target particle recoiling from a scattering event has high kinetic energy compared with potential energies with neighboring particles. This is an excellent assumption for x-ray Compton scattering studies of electronic momentum distributions in solids, and for electron scattering studies of subtructure of nucleons in high energy physics. The IA incoherent structure function $S(Q,\omega)$ has a simple integral relation to single-particle momentum distribution $n(p)$. The Compton profile $J(Y,Q) \equiv QS(Q,\omega)$ is a universal function of a scaling variable

$Y \equiv (\omega - \hbar Q^2/2M)/Q$ and independent of Q [11]. For DINS from liquid ^4He, a condensate would produce a $n_o\delta(Y)$ peak in the Compton profile, corresponding to a peak in $S(Q,\omega)$ at the recoil energy $\omega = \hbar Q^2/2M$ with integrated intensity proportional to n_o. This prediction provides motivation to use DINS experiments to study the relation of Bose condensation and superfluidity in ^4He.

Unfortunately, this IA ideal can not be reached for liquid ^4He at any feasible Q due to *final state effects* (FSE). Even though experimental Q's can now reach deep into the DINS range, interactions of the recoiling helium atom with neighboring atoms broaden the Compton profile. This broadening may be represented as a convolution of $J_{IA}(Y)$ in Y with a FSE broadening function $R(Y,Q)$. The combination of a FSE theory and quantum many-body calculations of $n(p)$ yields quantitative predictions for neutron Compton profiles. The remarkable story of Monte Carlo and quantum many-body calculations of $n(p)$ has been told elsewhere [8,9]. In these proceedings, I emphasize developments in the theory of FSE, and the comparison of recent DINS experiments to theory.

The first physical picture of FSE was presented by Hohenberg and Platzman [10] in 1966. A helium atom recoiling from a neutron scattering event has a collision lifetime with neighboring atoms, $1/\tau = \hbar Q\rho\sigma(Q)/M$. Here ρ is density, $\sigma(Q)$ is the He-He cross section and M is mass. $R(Y,Q)$ would be a Lorentzian in Y of width $\Delta Y = \rho\sigma(Q)$. If the ^4He-^4He potential had a hard core, such that $\sigma(Q)$ went to a constant at high Q, the Compton profile would obey Y-scaling without satisfying the IA. The IA would not be valid no matter how high the Q. The actual $\sigma(Q)$ has been measured and found to decrease slowly with increasing Q (approximately logarithmically), modulated by 'glory' oscillations resulting from quantum interference between identical particles. The corresponding potential is steeply repulsive at short distances. The IA would be approached equally slowly with increasing Q, while the required instrumental energy resolution would scale as $\Delta\hbar\omega \propto Q^{-1}$. The corresponding required neutron intensity increases approximately as Q^3 for most spectrometers providing an intensity limit to the achievable Q.

However, this Lorentzian broadening FSE theory disagrees with experiment even for the normal fluid where the PIMC prediction for $J_{IA}(Y)$ is approximately Gaussian except as it tails off at large $|Y|$. Normal fluid experiments are within a few % of the PIMC-IA prediction. The Lorentzian FSE theory predicts too much broadening as well as Lorentzian tails decreasing as $O(Y^{-2})$ at large $|Y|$ that are not observed. A Lorentzian $R(Y,Q)$ would also violate the kinetic energy sum rule which requires the second moment of the Compton profile to have the IA value. Thus, the sum rule requires the second moment of $R(Y,Q)$ in Y to be zero.

Another approach to FSE has been to develop additive corrections to the IA as a truncated power series in inverse powers of Q [12,13]. The first term in this expansion is the IA. The next term decreases as Q^{-1} and involves the semi-diagonal two-body density matrix $\rho_2(r,r";r',r")$. It is natural (although, we shall learn later, incorrect) to assume that only the first few terms in this series are important at high Q, and therefore that FSE fall off as $O(Q^{-1})$. No such additive corrections to the IA can cancel a Y-scaling Bose condensate δ-function.

The empirical failure of the Lorentzian broadening theories in the normal fluid and the additive correction FSE theories decreasing as $O(Q^{-1})$ encouraged investigation of $n(p)$ by DINS at increasingly large Q [14]. Early reactor neutron experiments with their thermal neutron spectrum could not practically exceed $Q = 12\AA^{-1}$. But the advent of pulsed spallation neutron sources in the 1980's with their high flux of epithermal neutrons enabled practical experiments at Q's up to $30\AA^{-1}$, well into the DINS range.

Unfortunately, as we shall see, Nature frustrates any hope that FSE could be ignored at any feasible momentum transfers Q. The correct qualitative physics of FSE was first identified by Gersch and Rodriguez [15] (GR) in 1973. The positions of atoms in the ground state of liquid ^4He are correlated as described by their radial distribution function $g(r)$. They stay away from the repulsive core of neighboring atoms in order to minimize their energy. A high kinetic energy ^4He atom recoiling from a neutron collision must travel a distance on the order of the first peak ($\approx 3\AA^{-1}$) in the radial distribution function before it begins to scatter at the rate $1/\tau$ of the Hohenberg-Platzman theory. This significantly reduces FSE, but it does not eliminate them. FSE still scale like the cross section $\sigma(Q)$. The GR quantitative calculation of FSE used an eikonal approximation for the scattering, a novel cumulant expansion of $S(Q,\omega)$ involving again the semi-diagonal two-body density matrix ρ_2, and an approximation to ρ_2 in terms of the one-body density matrix $\rho_1(r, r')$ and the radial distribution function $g(r)$. The resulting FSE broadening function $R(Y, Q)$ is non-Lorentzian with a central peak for small $|Y|$, rapidly damped oscillations at large $|Y|$, and a zero second moment in Y as required by the kinetic energy sum rule.

Actually, the above description is a paraphrase in modern language of what GR accomplished. Their work was perhaps 15 years ahead of its time, phrased in different language, and largely ignored. One can speculate about the reasons. It was published prior to the realization of the general character of Y-scaling in all Compton scattering (or deep inelastic scattering) experiments throughout physics [11]. It appeared at a time when the only experiments had been performed at the low Q's of reactor sources, and Monte Carlo and variational calculations of $n(p)$ were not accurate. Their quantitative predictions were buried in an experimental paper which claimed to measure $n_o \simeq 0.02$, in disagreement with both many-body theory and all subsequent experiments. Their step function approximation to the radial distribution function is unrealistic. The approach did not make contact with the more familiar methods of diagrammatic perturbation theory. In retrospect, their quantitative theory underestimated the FSE broadening.

In 1987-89 the author [16] (S) developed a new approach to FSE using a Liouville projection superoperator expansion of $S(Q,\omega)$ about the ground state wave function. The superoperator projected all single particle excitations of momentum transfer $\hbar Q$ above the ground state. The expansion was truncated at the level of ρ_2, which again is approximated in terms of the $g(r)$ and ρ_1 in a somewhat different manner than GR. Although the expansion generates many terms, all terms which did not Y-scale in the asymptotically high Q limit for hard core potentials are dropped. The theory has a perturbative representation as a Dyson equation in which FSE are vertex corrections involving additional single particle excitations. The two-body t-matrix is approximated by semiclassical methods which are accurate at high Q. The small parameter is a product of the t-matrix and ρ_2 which is well behaved. The Dyson equation corresponds to an infinite order partial resummation of the additive FSE correction series. This resummation has an entirely different asymptotic Q dependence than the first correction to the IA in the additive series.

The result is, like the GR theory, a convolution broadening $R(Y,Q)$ of the IA Compton profile $J_{IA}(Y)$. Moreover, it may be described by a simple physical picture. The scaling variable Y is canonically conjugate to the distance traveled by a recoiling ^4He atom. The FSE broadening function $R(Y,Q)$ is the Fourier transform of the classical scattering probability of no collisions as a function of this distance. This probability depends on real space correlations in the ground state wave function through the radial distribution function. The inputs required to calculate FSE are all known from experiment, so the theory has no adjustable parameters. The central peak of $R(Y,Q)$ is about twice as wide in Y as the GR calculation. FSE effects on the normal fluid Compton profile are very small in agreement with experiment, because the IA profile is almost Gaussian and FSE do not alter the second moment of the Compton profile. But for the superfluid where the IA Compton profile is very non-Gaussian, the FSE broadening is sufficient to eliminate the distinct Bose condensate δ-function peak predicted by the IA. The Q dependence follows $\sigma(Q)$, so that FSE decrease very slowly with increasing Q.

My theory appeared a year or two before the high Q experiments from the new generation of pulsed spallation neutron sources. These beautiful experiments are best described in the aforementioned review by Snow and Sokol [6] to which we refer readers. After correcting the data for instrumental effects such as resolution and backgrounds, there is almost perfect agreement within statistical error between experiment at $Q = 23\mathring{A}^{-1}$ and ab initio predictions for $J(Y,Q)$ obtained by combining GFMC and PIMC $n(p)$ with the author's theory for FSE [16]. This is true even though the shape of the Compton profile varies significantly with temperature, becoming more sharply peaked and less Gaussian as lower temperatures. As $g(r)$ changes little in this range, the same $R(Y,Q)$ can be used at all temperatures to a good approximation apart from a simple linear scaling of the Y variable with density. Thus the experimental data are consistent with calculations that predict a Bose condensate fraction $n_o \approx 10\%$. The forward prediction of experiment by S-PIMC and S-GFMC theory is quite good at high Q [17].

Detailed comparisons with other FSE theories can be made assuming the $n(p)$ calculations are correct [18]. There is dramatic disagreement with the IA theory at superfluid temperatures especially in the region near $Y = 0$ where the condensate would contribute. There is similar disagreement with additive FSE corrections that allow a condensate δ-function to persist. The broadening predicted by GR is about a factor two too small.

Not everything is perfect, however. One unexplained discrepancy is a slight asymmetry in which the $Y \ll 0$ ($Y \gg 0$) side of the Compton profile is slightly lower (higher) than experiment [6]. The agreement is not so good at smaller Q [19], as should be expected from the approximations employed. These discrepancies point to the need for further development of the DINS theory.

The inverse problem of extracting $n(p)$ and $R(Y)$ from experiment in the presence of noise, instrumental broadening, and backgrounds is ill-posed and more difficult. One approach is to assume the FSE theory to be correct, and to fit a model form for $n(p)$ that includes a Bose condensate with n_o as a parameter along with other known singular structures induced by the condensate. Using this model fitting approach, Snow and Sokol [6] report broad trends in the extracted values for n_o and the kinetic energy as functions of temperature and density that are in reasonable agreement with expectations. However, the error bars on n_o are approximately $\pm 2\%$ which are not small compared to n_o itself. With those errors it is impossible to say with precision that there is evidence for a sharp transition from zero to non-zero n_o as the temperature is lowered past T_λ. Indeed, the data below T_λ may also be adequately fit by $n(p)$ that is a sum of narrow and wide Gaussians that have no δ-function. Attempts to extract $R(Y, Q)$ assume, conversely, that the GFMC and PIMC calculations of $n(p)$ are correct. The result is reasonably close to my theory at high Q, although there are differences in the damped oscillatory wings at large $|Y|$. There is no estimate of the statistical significance of those differences.

The most serious theoretical criticism of the my approach to FSE has addressed the approximation to the semi-diagonal two-particle density matrix ρ_2. Ristig and Clark [20] in 1989 pointed out that the my approximation, while satisfying the $p-$ and $q-$ sum rules on ρ_2, does not satisfy other known properties such as symmetry and sequential relations. The different approximations of GR and by Rinat [21] also satisfy these properties to a limited extent. Ristig and Clark suggest a general structure for ρ_2 based on hypernetted chain theory which satisfies all the known constraints including sum rules, symmetry and sequential relations. Unfortunately, this form has not yet been quantitatively used in my theory.

Carraro and Koonin (CK) in 1990 [22] presented a calculation of FSE that did not depend on approximations to ρ_2. They solved the scattering problem of a high Q recoiling atom moving in the instantaneous potential of a Jastrow approximation to the many-body wave function, the assumption being that neighboring atoms provide a static field. Their resulting $R(Y, Q)$ has approximately the same width central peak as I predicted at high Q, and so they also agree well with experiment. There are some differences between the two predictions in the damped oscillatory wings at large $|Y|$, but the available experiments are insensitive. They also predict a more severe Q dependence, but the discrepancies between of both CK and S theories with experiment increase at small Q and are comparable in magnitude.

In 1996 Mazzanti et al. [23] reexamined the GR theory using an HNC estimate for the semi-diagonal two-body density matrix ρ_2 based on the earlier work of Ristig and Clark. They claim essential agreement between the GR, CK and S predictions for the width of the central peak of $R(Y, Q)$ provided that a proper ρ_2 is used in GR theory. Experiments are insensitive to somewhat larger differences between theories in the damped oscillatory wings at large $|Y|$. In the original GR paper, their ρ_2 relied on a step function approximation to $g(r)$ at $r_o = 2.5\mathring{A}$ which gave too little FSE broadening. Mazzanti et al. note that a choice of $r_o = 2.1\mathring{A}$ in the original theory would also yield good agreement with experiment and the CK and S theories for $R(Y, Q)$. However, examination of the measured $g(r)$ reveals that there is almost no probability for collisions at $r = 2.1\mathring{A}$.

Thus, today there are three different theoretical approaches that are in quantitative agreement about the magnitude and character of FSE at high Q. What remains to be tested is whether use of a better ρ_2 in my theory would significantly alter its prediction.

A focus of recent experimental work has been systematic studies as a function of Q [19,24]. Andersen et al. [24] in 1994 measured the FWHM (full-width-half-maximum) and peak position of $S(Q, \omega)$ in the range $3 \leq Q \leq 12\mathring{A}^{-1}$. They observe at least four oscillations in the FWHM and peak position in both the normal fluid and the superfluid that appear to track the aforementioned glory oscillations of the He-He cross section. Their interpretation is that it provides model-independent evidence that final state effects are present in the data which vary like $\sigma(Q)$. However, the Q's are not large enough to ignore coherent scattering. The shift in peak position also suggests there are real part of the self-energy corrections to the IA in addition to the vertex corrections associated, in my theory, with FSE broadening.

The most significant attempt to use Q-dependent data has been by Glyde and coworkers [25]. They fit the dynamic structure function to a cumulant expansion in the Fourier transform of Y (to paraphrase) using up to sixth order cumulants. They claim to separate the contributions from the IA and FSE by their differing Q dependencies. For example, we know that the second cumulant (moment) of the Compton profile is independent of FSE. But in the fourth moment the IA contributions are independent of Q varying as the fourth cumulant of $n(p)$, while the FSE contribution varies as Q^{-2} with a coeffecient. proportional to the force-force correlation function. They claim to observe just such Q dependencies in the data. Such fits are used to simultaneously infer $n(p)$ and $R(Y,Q)$.

Two comments on this approach may be offered. First, if ^4He had a hard core potential, there would be no way to separate the IA and FSE contributions using differing Q-dependences as they would both Y-scale. The cumulant expansion would not converge, e.g. in the fourth moment the force-force correlation function would be infinite as it would be the expectation of products of two δ-functions. Although the real He-He potential may not be hard core, it is steeply repulsive such that this cumulant expansion should converge slowly at high Q. It seems unlikely that only a few terms in the expansion provide an adequate description. This discussion is obviously related to the earlier controversy regarding additive vs. convolution theories of FSE. Second, prior work by Sokol and collaborators has found statistical evidence for the adequacy of a two Gaussian description of $n(p)$. The data analyzed by Glyde et al. are not dramatically better, so the claim to determine many more parameters seems inconsistent.

"Where there's smoke, there's fire." This old adage is good enough for me. I am sure about the correlation between Bose condensation and superfluidity. The empirical manifestations are overwhelming. We have achieved excellent quantitative agreement between *ab initio* theory and high precision DINS experiments. Further efforts to understand the 'smoke' should tell us more about the 'fire'. But for those who insist on "Seeing is believing!", a new approach other than DINS will be needed to directly observe a Bose condensate δ-function in the momentum distribution of superfluid ^4He.

ACKNOWLEDGMENTS

This research was funded by the U. S. Dept. of Energy. We acknowledge the Army Research Office for financial assistance to attend the Workshop on Condensed Matter Theories XX and the U. S. / India Joint Seminar on Bose Einstein Condensation and Pairing Phenomena in Pune, India where this paper was presented in December, 1996.

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