A novel method for the extraction of the condensate fraction of liquid $^4$He

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Abstract

We present a new, semi-phenomenological method to extract the condensate fraction $n_0(T)$ from two sets of measured responses of $^4$He with identical kinematics at $T < T_c$ and $T > T_c$. 
I. INTRODUCTION

Over the past decades attempts have been made to determine the condensate fraction $n_0(T_\prec)$ of liquid $^4$He, which is defined as the asymptotic limit of the single-atom density matrix (SADM) $\rho_1(0, s; T_\prec)/\rho(T_\prec)$.

$$n_0(T_\prec) = \lim_{s \to \infty} \frac{\rho_1(0, s; T_\prec)}{\rho(T_\prec)}$$

$\rho(T) = \rho_1(0, 0; T)$ is the number density. We shall use the notation

$$T_\prec = T < T_c; T_\succ = T > T_c; T_\succsim = T_\prec, T_\succ$$

In spite of the increasing quality of data, the various experimental results show an unsatisfactory spread in $n_0$. The reason may well be that there is no unequivocal, direct link between the above definition of $n_0(T_\prec)$ and experimental information. The quality of an extracted condensate fraction thus depends on the accuracy of the approximate isolation of the relevant SADM, which contains the condensate fraction.

Without striving for completeness we briefly review:

i) computations from first principles;

ii) results from the comparison of specific theories and data;

iii) data analysis with minimal theoretical input;

We then propose and evaluate a novel extraction method which, except for minor assumptions, is largely model-independent.

*Computations:* In principle stochastic methods for a representative sample of a finite number of atoms determine the ground state wave functions and thus $\rho_1$. Those wave functions, and thus the SADM, can be computed up to large values of $s$ and thus directly provide $n_0$ (see for instance [1,2]). In practice the method is accurate only for $T = 0$ K, and from sufficiently large $s$ one extracts $n_0(T = 0)$. Nevertheless, even for $T = 0$, different stochastic methods produce a spread in $n_0$ of, as much as 25% [3].

For finite $T$ a calculation of $\rho_1$ requires a canonical average
\[
\rho_1(0, s; T)/\rho(T) = Z^{-1}(\beta) \int d\mathbf{r}_1 \left( \Pi_{k \geq 2} \int d\mathbf{r}_k \right) \langle \mathbf{r}_1, \mathbf{r}_k | \exp[-\beta H_A] | \mathbf{r}_1 - s \hat{\mathbf{i}}_z, \mathbf{r}_k \rangle
\]

(2)

with \( Z(\beta) \), the partition function.

Results for \( \rho_1(0, s; T \neq 0) \) known to us, are for \( s \lesssim 7 \text{Å} \) and for a number of discrete \( T_c \) around \( T_c \), but beyond \( s \approx 2.5 \text{Å} \) the computed SADM apparently have sizable inaccuracies. This reflects on condensate fractions, which have been extracted from \( s \) in the range \( \approx 4 - 7 \text{Å} \) where a constant value of the SADM is only reached on the average.

**Theory:** Efforts to obtain the condensate fraction naturally focus on the extraction of the SADM from an observable. A prime example is the cross section for inclusive neutron scattering on He, which is proportional to the response \( \phi(q, y) \). The latter is a function of two kinematic variables, e.g. the momentum transfer \( q \) and the GRS-West scaling variable, \( y = (M/q)(\nu - q^2/2M) \), with \( M \), the mass of an atom. For fixed \( q \) the variable \( y \) is a measure for the energy loss \( \nu \).

In order to compare with experiment the above response has to be folded into the experimental resolution function \( E \). One may then formally write the response and its Fourier Transform (FT) in a closed form (see for instance Ref. [4,6,7])

\[
\phi^{th,conv}(q, y; T) = \int dy' \int dy'' F_0(y'; T) R(q, y - y'; T) E(q, y' - y''; T)
\]

(3a)

\[
\tilde{\phi}^{th,conv}(q, s; T) = \int dy \exp[-isy] \phi^{th,conv}(q, y; T) = \tilde{F}_0(s; T) \tilde{R}(q, s; T) \tilde{E}(q, s; T)
\]

(3b)

The first factor \( F_0(y; T) \) is the asymptotic limit of the response, and depends on the single-atom momentum distribution \( n(p, T) \). Its Fourier Transform is just the SADM. Final State Interactions (FSI) are formally contained in \( R \), which can be expanded in powers of \( 1/q \) and which depends on higher order density matrices \( \rho_n \). In practice it suffices to retain only the dominant FSI \( \propto \rho_2/q \). Finally, \( E \) is Experimental Resolution (ER) of the measuring devise.

In the standard approach one computes from dynamics the FSI factor \( R \), which modifies the asymptotic response \( F_0 \) for finite \( q \) (see for instance Ref. [4,6,7]). In addition many-body density matrices which weigh all components are required. We focus on \( F_0 \), which is related to the momentum distribution \( n(p; T) \) and which for \( T_c \) requires modeling.
\[ n(p, T_\leq) = n_0(T_\leq)[(2\pi)^3 \delta(p) + f(p; T_\leq)] + A(T_\leq)n^{\alpha_0}(p; T_\leq) \]
\[ A(T_\leq) = 1 - n_0(T_\leq)[1 + \tilde{f}(0; T_\leq)] \]  \hspace{2cm} (4)

In the above parametrization \( n_0(T_\leq) \) one finds in addition to the macroscopic fraction \( n_0(T_\leq) \) of atoms with momentum \( p = 0 \), \( f(p, T_\leq) \), the fraction of atoms relative to \( n_0 \) with momenta \( p \lesssim p_c \) in the immediate neighborhood of \( p = 0 \). Finally, \( n^{\alpha_0}(p, T) \) above is the normal part of the momentum distribution of atoms with \( p \gtrsim p_c \); \( A(T) \) cares for proper normalization.

Albeit dominant for \( p \neq 0 \), \( n^{\alpha_0}(p, T_\leq) \) is not directly measurable and is for low \( T \) frequently assumed to be \( T \)-independent: \( n^{\alpha_0}_0(p; T_\leq) \leftrightarrow n^{\alpha_0}_0(p; T_\geq) = n(p; T_\geq) \). For \( T_\geq \) it is the measurable \( n(p; T) \). Equivalently for the SADM

\[ \rho_1(0, s; T_\leq)/\rho(T_\leq) = n_0(T_\leq) + G(s; T_\leq) \]  \hspace{2cm} (5a)
\[ G(s; T_\leq) = n_0(T_\leq)\tilde{f}(s; T_\leq) + A(T_\leq)[1 + \tilde{f}(0, T_\leq)]\rho^{\alpha_0}_1(s; T_\leq)/\rho(T_\leq) \]  \hspace{2cm} (5b)

Above, \( G \) is the difference between the SADM and its asymptotic limit \( n_0 \), which will be called the deficit function. By definition \( \lim_{s \to \infty} G(s, T_\leq) = 0 \).

We summarize: Except for \( T = 0 \), there is no accurate information on the SADM for large \( s \). For finite \( s \) an expression for \( G \), e.g. \( (5b) \), is model-dependent and without knowledge of both \( \rho_1(0, s; T_\leq) \) and \( n_0(T_\leq) \) there is no accurate way to reach the deficit function \( G \).

\textit{Data – analysis}: One method used in the past relates the integral of the difference between responses for \( T = T_\geq \) in the region \( y \approx 0 \) to the fraction of atoms having momenta in that region. The method is not accurate because of imprecise isolation of FSI and ER broadening in \( \rho_1 \) (see for instance Ref. \( [9] \)).

Of similar nature are cumulant parametrizations of responses for \( T_\leq \). Even if the above assumption on \( n^{\alpha_0}(p, T_\leq) \) is made, the data do not permit the extraction of an accurate value of \( n_0(T_\leq) \) and \( p_c \). Instead one studies fits for varying \( n_0(T_\leq) \).
II. CONSISTENCY RELATIONS AND A NOVEL METHOD FOR THE EXTRACTION OF THE CONDENSATE FRACTION.

We now describe a new method for the extraction of the condensate fraction as it appears in the SADM for $T_\prec$. We try to avoid the described insufficient information on the latter by exploiting data on inclusive scattering on two $T_\prec$ at precisely the same momentum transfer $q$ and energy loss $\nu$, or the related scaling variable $y$. Fairly recent data of that type exist for $T = 1.6, 2.3$ K\textsuperscript{12,13} (MARI data).

We first define from Eq. (3b) the ratio of the FT of those corresponding data

$$\eta^{\text{exp}}(q, s; T_\prec, T_\succ) \equiv \left[ \frac{\tilde{\phi}_E(q, s; T_\succ)}{\phi_E(q, s; T_\prec)} \right]^{\text{conv}} = \left[ \frac{\tilde{\phi}(q, s; T_\succ)}{\phi(q, s; T_\prec)} \right]^{\text{deconv}} \quad (6a)$$

$$\approx \frac{\rho_1(0, s; T_\succ)/\rho(T_\succ)}{\rho_1(0, s; T_\prec)/\rho(T_\prec)} \quad (6b)$$

Eq. (6a) expresses the $T$-independence of the ER for the MARI data and as a consequence the ratio of actual convoluted data are replaced by deconvoluted ones. Those $\eta^{\text{exp}}$ depend on $q$ and are complex, because the FT of the data are complex.

Eq. (6b) is of a different nature. It assumes that the FSI function $R$ is at most weakly $T$- dependent. Although verified within the accuracy of the data\textsuperscript{14}, we cite weak $T$-dependence on the measured pair-distribution function $g(r, T)$\textsuperscript{13} which, at least in some theories, enters the FSI function $R$\textsuperscript{4}. The price for ‘removing’ $R$ and the ER is the appearance of two SADM, instead of the desired $\rho_1(0, s; T_\prec)/\rho(T_\prec)$.

Since the precision with which one ultimately extracts the condensate fraction depends on the quality of the input, we discuss the latter. We note that $\eta^{\text{exp}}$ in (6) uses not actual data, but instead their FT. With substantial noise, in particular in the larger $y$ tails of the data for $\phi(q, y)$, one cannot avoid smoothing, or even cutting out those low-intensity data, which affect the accuracy of $\eta^{\text{exp}}$.

We first apply the method to the above-mentioned MARI data at $T_\prec = 1.6$ K; $T_\succ = 2.3$ K\textsuperscript{13} from which we chose a representative sample of highest quality for which $q = 17, 21, 23, 29\text{Å}^{-1}$. From those we extract the ratio $\text{Im}[\eta^{\text{exp}}(q, s)]/\text{Re}[\eta^{\text{exp}}(q, s)]$, which is well
determined in the range $s \lesssim 2.5 \text{Å}$. For growing $s$, the imaginary part increases from 0 but is, even at medium $s \approx 2.5 \text{Å}$, only 2% of the real part, and can thus for all purposes be neglected. This confirms that at least the ratio of the involved FSI functions $R$ is virtually $T$-independent.

Next we investigate the $q$-dependence of $\text{Re}[\eta^{\exp}]$ and show in Fig. 1 data for some individual $q$. Before judging the quality we mention that, contrary to predictions, some data for $T_\triangleright$ and varying $q$, and more for $T_\triangleleft$, are not uniformly smooth in $q$. This may cause apparent $q$-dependence in $\eta$ and justifies the use of an average for $s \lesssim 2.5 \text{Å}$

$$\eta^{\exp, \text{av}}(s; T_\triangleright) \equiv \left\langle \eta^{\exp}(q, s; T_\triangleright) \right\rangle_q \approx \left\langle \text{Re}[\eta^{\exp}(q, s; T_\triangleright)] \right\rangle_q$$  \hspace{1cm} (7)
As a first step we test (6b) with the only available computed results on SADM for $T_\geq 3$. Without any dynamical cause, the outcome for $T=1.54$ K closest to $T=1.6$ K of the MARI data, is not very close to values from interpolation between neighboring $T$. We suspect the mentioned inaccuracies which are also apparent in non-vanishing condensate fractions for $T_>$ and the non-smooth dependence of $n_0(T_\leq)$ as function of $T$ outside their estimated theoretical error bars. Nevertheless we use interpolated computed results and define for $T_\leq = 1.6$ K; $T_> = 2.3$ K

$$\eta^{\text{comp}}(s; 1.6, 2.3) \equiv \left[ \frac{\rho_1(0, s; 2.3)/\rho(2.3)}{\rho_1(0, s; 1.6)/\rho(1.6)} \right]^{\text{comp}}$$

The above as function of $s \leq 2.5\text{Å}$ is also entered in Fig. 1 and is seen to represent the data rather poorly. We shall thus exclusively use $\eta^{\text{exp,av}}$ and return to Eq. (5a), which by means of (7) and (6b) becomes

$$n_0(T_\leq) = \frac{\rho_1(0, s; T_>)/\rho(T_>)}{\eta^{\text{exp,av}}(s, T_\leq)} - G(s; T_\leq)$$

We note that, contrary to (1), Eq. (9) is not applicable in the asymptotic region, because in order to produce a constant, numerator and denominator in the ratio in (9) have to tend to zero in exactly the same fashion. This is an impossibly stringent demand.

Although Eq. (9) provides in principle a value of the condensate fraction for arbitrary, finite $s$, it is clearly of greater interest to consider a range of $s$. In fact, the right hand side of (9) is a function of $s$, whereas the left hand side is a constant, implying a consistency test, to be passed as a condition for a successful extraction of $n_0(T_\leq)$. The size of the $s$-range depends on the available information on the various functions in (9).

The most delicate source of information is the deficit function $G$. After the warnings above, one clearly does not want to use (5b) and has thus to rely on the model-independent, not too accurate results of Ref. [3], which for $4 \lesssim s(\text{in Å}) \lesssim 7$, provide $n_0(T)$ with uncertainties of the order of 15%. The crucial point is that those uncertainties decrease relatively to $G(s; T_\leq)$ which increases for decreasing $s$. We thus conclude that, up to medium $s \lesssim 2.5\text{Å}$, one can trust and use the computed $G$. The above happens to also be the range for which the available data determine $\eta$ sufficiently well.
We thus perform the consistency test, implied by (8) and it comes as a surprise that the right hand side in the considered $s$-range is only weakly $s$-dependent, leading to

$$n_0(1.6) = 0.0625 \pm 0.0017$$

$$n_0(0) = 0.090 \pm 0.030$$

(10)

The latter is the result for a standard extrapolation to $T = 0$. The small error limits are due to averaging results for different $s$; we could not estimate the same for uncertainties in $G$. We note that the errors on the three functions in (9) are uncorrelated, which underscores the reliability of the extracted value of $n_0(T_\prec)$.

The above numbers use $G(s; T = 1.6K)$, interpolated between values for $T= 1.54, 1.82K$ as reported by Ceperley. We mentioned that the former set, does not interpolate smoothly between values for $T=1.18, 1.82 K$. Smoothing leads to a lower condensate fraction. Obviously the accuracy with which one can extract the condensate fraction depends on the same for the input.

Above we also listed older Argonne data for fixed $q = 23.1Å^{-1}$ and some 10 temperatures around $T_c$. Unfortunately we do not have available the actual data and the ER functions, and have to analyze instead parametrizations of the above, as given by the authors. Those are given by the authors in the form of double Gaussians for data deconvoluted from ER, and in addition also deconvoluted from FSI. The information no doubt reduces the required accuracy. Yet, in view of scarcity of information we performed the above analysis for the Argonne data. In order to compare with the MARI data and we fix $T_\succ$ at 2.3 K.

One first observes that the computed FT of the above parametrized data are essentially real. Next, ratios of those FT for and $T_\prec$ and the above $T_\succ$ are identical within 1%, in support of (9). Nevertheless, only a limited part of the information can be used for an analysis of the above type. Thus for $T_c \geq T \gtrsim 1.8 K$, $n_0(T_\prec)$ is the difference of nearly equal terms in (9). A reliable determination requires a precision on $\rho_1(0, s; T_\succ)/\rho(T_\succ)$ and $G(s; T_\prec)$, which is beyond the Ceperley results. A different difficulty occurs for $T \lesssim 1 K$, where one has to make an uncertain extrapolation, using the lowest $T$ results of Ceperley.
The following outcome

\[ n_0(T = 1.0 \text{ K}) = 0.063 \pm 0.006 \]
\[ n_0(T = 1.5 \text{ K}) = 0.060 \pm 0.008 \]
\[ n_0(T = 1.8 \text{ K}) = 0.050 \pm 0.005 \]  

(11)
carries some 20-25\% uncertainties, which appreciably exceed the one in (10) based on the MARI data. One notes that \( n_0(T \approx 1.6 \text{ K}) \) from the MARI and Argonne data approximately agree. However, in view of the fact that we had to use parametrizations of the Argonne data, we do not attach too much significance to the correct trend of \( n_0(T) \) as function of \( T \) and the somewhat low, but not unreasonable, average \( \langle n_0(T = 0) \rangle_{T <} = 0.079. \)

In conclusion, we have suggested and worked out a new method to extract the condensate fraction in \(^4\text{He}\) from the Fourier transforms of data sets on structure functions at the same momentum and energy transform, but for two \( T \) below and above \( T_c \). In addition the method requires some previously computed dynamical information. The expression (9) for \( n_0(T <) \) appears in principle as a function of \( s \), but is in practice a well-determined and thus meaningful constant, the condensate fraction.
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Figure Captions