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DETERMINATION OF MOMENTUM DISTRIBUTIONS FROM DEEP INELASTIC NEUTRON SCATTERING EXPERIMENTS - A BAYESIAN STUDY

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ABSTRACT

A Bayesian analysis shows that the determination of momentum distributions in quantum fluids and solids by deep inelastic neutron scattering is an extremely ill-posed problem. The argument is illustrated with the issue of the Bose condensate fraction in superfluid ^4He.

INTRODUCTION

There is a long history of experiments [1] aimed at measuring the momentum distributions in quantum solids and fluids by neutron scattering at high energy and momentum transfers, which is termed "deep inelastic neutron scattering" (DINS). Undeniably experiment can distinguish between various theoretical models for the neutron scattering law. However, the goal of the present paper is to show that the inverse problem of extracting $n(p)$ from the experiment is extremely ill-posed. For example, analyses of such experiments on superfluid ^4He [2] have claimed to confirm the existence of a Bose condensate fraction, n_0, and to determine its value. We show that available data are also consistent with $n_0=0$, and that available determinations of n_0 should be regarded as model-dependent.

BAYES' THEOREM

All data analysis methods for determining $n(p)$ are, at least implicitly, based on Bayes' theorem. This is expressed in terms of the probability density function (p.d.f.), $P[n(p)|D(Y)]$, which is the conditional probability of the momentum distribution, $n(p)$, given the data, $D(Y)$. Bayes' theorem states that

$$P[n(p)|D(Y)] \propto P[D(Y)|n(p)] \times P[n(p)] \quad . \qquad (1)$$

Here, $P[n(p)]$ represents our state of knowledge about $n(p)$ (or the lack of it) before we have any data - this is referred to as the *Prior* p.d.f. The data modify our prior state of knowledge through the term $P[D(Y)|n(p)]$, which is the probability of obtaining the measured data for a given momentum distribution - this is referred to as the *Likelihood* function. In the limit of independent Gaussian statistics, the Likelihood function reduces to the familiar form

$$P[D(Y)|n(p)] \rightarrow \exp(-\frac{\chi^2}{2}) \quad . \qquad (2)$$

The product of the Likelihood and the Prior p.d.f. is proportional to $P[n(p)|D(Y)]$ the *Posterior* p.d.f., or our state of knowledge after we have measured the data. Our best estimate of $n(p)$ is given by the maximum of the Posterior p.d.f., and the reliability (error estimate) is given by its width.

Different data analysis procedures correspond to different choices for the Prior p.d.f. $P[n(p)]$.
For example, the conventional procedure to determine n_0 in ^{4}He [2] assumes a particular model for $n(p)$ with a few parameters based on the physics of the problem, e.g. the terms in $n(p)$ proportional to n_0 involve a delta function plus associated $1/p^2$ and $1/p$ singularities. Another procedure is to arbitrarily assume a functional form for $n(p)$, such as a sum of two Gaussians. In either case, the parameters are estimated by maximizing the Posterior p.d.f. $P[n(p)|D(Y)]$. If the Prior p.d.f., $P[n(p)]$, is assumed to be a uniform function of those parameters, this is equivalent to the familiar procedure of minimizing χ^2 (i.e. maximum likelihood). Such data analysis procedures beg the question of whether the choice of Prior p.d.f. was correct. For example, how far out in p do the $1/p^2$ and $1/p$ singularities extend [3], or is there physical justification for $n(p)$ to be the sum of Gaussians? If the χ^2 for either method is acceptable, then the data shed no light on such questions. An alternative data analysis procedure is to deconvolve the data to obtain $n(p)$ which uses a different Prior p.d.f. For example, in the maximum entropy method [4] the Prior p.d.f. is taken to be the exponential of the entropy of $n(p)$ relative to a default model, which may for example be a numerical simulation of $n(p)$.

Regardless of the choice of Prior, it is the Likelihood function which incorporates the information contained in the data and it is the Likelihood function which can be evaluated exactly in terms of the experimental parameters. If the Likelihood function is a sharply peaked function of $n(p)$, then it will dominate the Posterior, i.e. no matter what our prior state of knowledge, the data force us towards the same choice of $n(p)$. If the Likelihood function is a broad function of $n(p)$, then the data have little effect on our state of knowledge and hence, the Posterior will depend crucially on the Prior. Fig. 1 shows a section through a schematic Likelihood function. The data constrain the distribution well in some directions (e.g. $n(p_2)$) but poorly in others (e.g. $n(p_1)$). The good directions are associated with large eigenvalues of the Log-Likelihood matrix ($\nabla\nabla\chi^2$), and the bad directions with small eigenvalues. In order to see how much information DINS data contain, we consider the sharpness, or otherwise, of the DINS Likelihood function.

ANALYSIS OF DINS EXPERIMENTS ON ^{4}He

In deep inelastic neutron scattering (DINS) experiments, the momentum distribution $n(p)$ is related to the experimental data, $D(Y)$, by

$$D(Y) = F_{IA}(Y) \otimes R_{expt}(Y) \otimes R_{FSE}(Y) + B(Y) + N(Y) \qquad (3)$$

Here " $\otimes$ " denotes convolution,

$$F_{IA}(Y) = n_0\delta(Y) + \frac{1}{4\pi^2 Q}\int_{|Y|}^{\infty} p\; n(p)\; dp \qquad (4)$$

is the impulse approximation (IA) prediction for the neutron scattering law (the Compton profile),

$$Y = \frac{M\omega}{Q} - Q/2 \qquad (5)$$

is the scaling variable, $R_{expt}(Y)$ is the spectrometer broadening function, $R_{FSE}(Y)$ is the broadening due to corrections to the impulse approximation such as final state effects (FSE) which may also depend on Q. $B(Y)$ is background, and $N(Y)$ is noise. The problem is to infer $n(p)$ given $D(Y)$.

Using Eqs. (3–5) one may calculate the Likelihood function. Fig. 2 shows the spectrum of eigenvalues for the DINS Likelihood function for ^{4}He under the conditions of the recent experiments of Sosnick, et al. [5], which epitomize the current state-of-the-art in DINS measurements. The $R_{FSE}(Y)$ was taken from the recent theory by Silver [6]. The continuous $n(p)$ was digitized into 92 pixels for $0 \leq p \leq 3.4$ Å^{-1}, hence 92 eigenvalues. We see that most of the eigenvalues are very small, indicating that the Likelihood function is flat in many directions. Thus, the problem is extremely ill posed in that many distributions will fit the data. This is particularly true at small p, which is primarily due to the form of the Compton profile, Eq. (4), rather than due to instrumental or final state broadening. Indeed, we already expect this to be true from the observation [5] that the Greens' Function Monte Carlo (GFMC) $n(p)$ [7] which does not have the correct singular behavior at small p, and the Hypernetted Chain $n(p)$ [8] which does have the correct singular behavior at small p, pro-

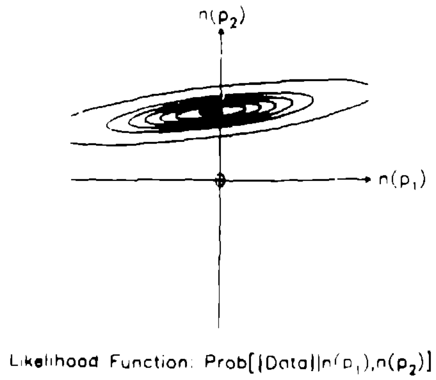

FIGURE 1 – A section through a schematic Likelihood function. The data constrain the distribution *n(p)* well in some directions but poorly in others. The good directions are associated with large eigenvalues of the Log-Likelihood function and the bad directions with small ones.

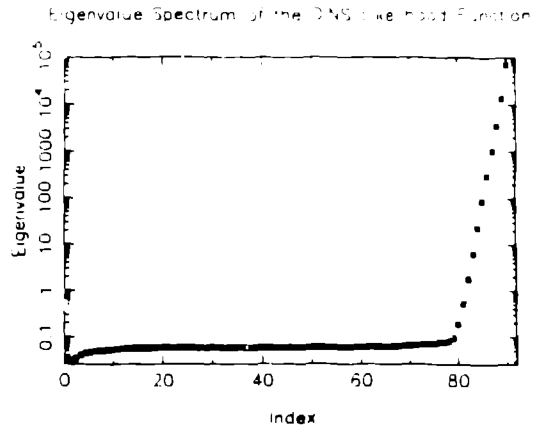

FIGURE 2 – The spectrum of eigenvalues for the Deep Inelastic Neutron Scattering (DINS) Likelihood function. Most of the eigenvalues are very small, indicating that the Likelihood function is flat in many directions.

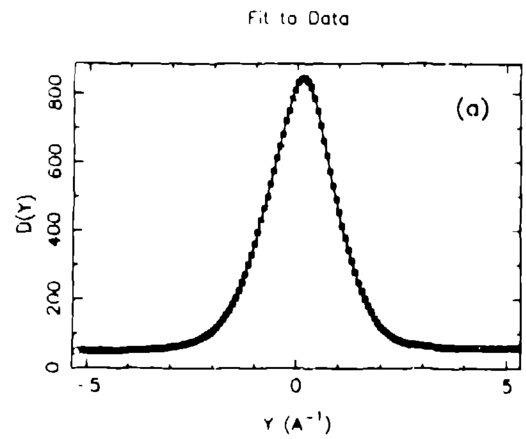

FIGURE 3(a) – *Simulated DINS data using the GFMC n(p)* (Whitlock & Panoff, 1988) shown as the dotted line in Figs. 3(b) & (c)., having a Bose condensate of 9.2%, with 100 times better statistics than that achieved in the state-of-the-art experiments of Sosnick, et al.

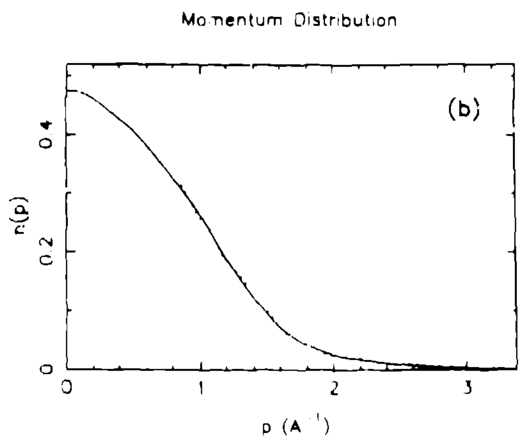

FIGURE 3(b) – Solid line is an *n(p)* which fits the simulated data in Fig. 3(a) with a 9.8% Bose condensate. Dashed line is the GFMC prediction, which was used to create the simulated data.

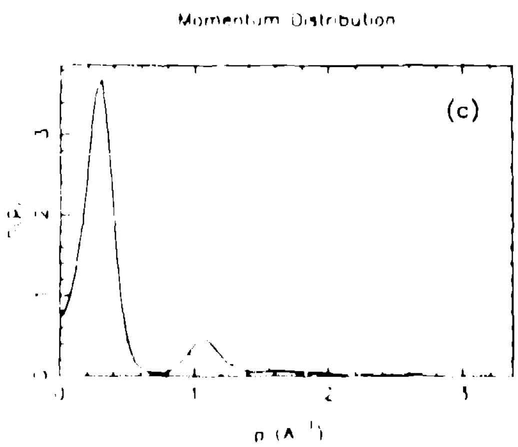

FIGURE 3(c) – Solid line is an *n(p)* which fits the simulated data in Fig. 3(a) with a 0% Bose condensate. Dashed line is GFMC.

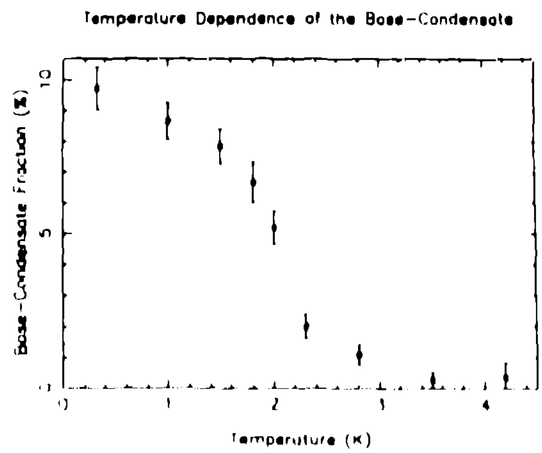

FIGURE 4 – The classical decrease of the Bose condensate fraction as ^{4}He is warmed through the λ-transition temperature. The DINS data were obtained by Sosnick, et al. (1988) and analyzed using an entropic prior with GFMC *n(p)* at T=0 K as default model.

duce almost identical predictions for $J(Y) = F_{IA}(Y) \otimes R_{expt}(Y) \otimes R_{FSE}(Y)$.

The ambiguity in inferring $n(p)$ from DINS data is illustrated graphically in Fig. 3 by a simulation. The mock data shown in Fig. 3(a) were created for the experimental conditions of Sosnick, et al. [5] with 100 times the number of neutrons achieved experimentally (ten times the statistical accuracy) using the GFMC $n(p)$ [7,9] as input. Figs. 3(b) and 3(c) show two very different $n(p)$ (continuous lines), both of which fit the data in Fig. 3(a). These were obtained by maximum entropy deconvolution [4] using as default models a best-fit Gaussian plus delta function for Fig. 3(b) and a best-fit Gaussian for Fig. 3(c) (which allows no Bose condensate). The GFMC had an n_o of 9.2%, to be compared with 9.8% for Fig. 3(b) and 0% for Fig. 3(c). Thus, data with statistical accuracy ten times better than currently achieved can not unambiguously establish the existence of a Bose condensate.

However, not all distributions allowed by the data make physical sense. Thus, we have extra prior knowledge, in the form of Physics, which constrains the allowed $n(p)$ much more tightly than the data alone. Fig. 4 shows such a determination of n_o, where the temperature dependent DINS data obtained by Sosnick, et al. [5] was deconvolved using an entropic Prior with the GFMC $n(p)$ (T=0 K) as the default model. The fact that n_o is found to be slightly greater than zero even above the λ-transition (although consistent with zero within errors) can be understood as a consequence of the bias of the default model toward the existence of a condensate.

CONCLUSIONS

The experimental DINS data [5] on ^{4}He show an obvious sharpening at small Y as the temperature is decreased below the λ-transition. Nevertheless, our counterexample shows that, despite prior claims to the contrary [1-2], the present generation of DINS experiments have not, and cannot be expected to, unambiguously establish the existence of a Bose condensate in ^{4}He. Prior knowledge in the form of a physical model is required to adequately constrain the inversion to determine n_o, and the available models [1-2] involve uncertainties [3] which would show up as systematic rather than statistical errors. The strongest evidence we have for the existence of a Bose condensate in ^{4}He is that *ab initio* calculations of $J(Y)$, including final state effects [6] and simulations of $n(p)$ [7-8,10], are in excellent agreement with DINS experiments [5] with no adjustable parameters, and these calculations predict the existence of a Bose condensate in ^{4}He at temperatures below the λ-transition.

More generally, the inversion of Compton profile data to extract $n(p)$ in any system is an extremely ill-posed problem, particularly at small p as can be seen from Eq. (4). Exceptional statistics, minimal final state broadening, and accurate instrumental resolution functions are required. For DINS on helium systems, it appears that significant final state broadening is unavoidable [6].

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