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AUTHOR(S): P. E. Sokol*
R. N. Silver, T-11/LANSCE
T. R. Sosnick**
W. M. Snow**

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*Department of Physics
The Pennsylvania State University
University Park, PA

**Intense Pulsed Neutron Source
Argonne National Laboratory
Argonne, IL

FINAL STATE EFFECTS IN LIQUID $^4$He: AN EXPERIMENTAL TEST

P.E. Sokol[†], R.N. Silver[‡], T.R. Sosnick[+], and W.M. Snow[+]

[†]Department of Physics, The Pennsylvania State University
University Park, PA

[‡]Theoretical Division, Los Alamos National Laboratory
Los Alamos, NM

[+]Intense Pulsed Neutron Source, Argonne National Laboratory
Argonne, IL

## INTRODUCTION

Inelastic neutron scattering at high momentum transfers can provide direct information on the atomic momentum distribution $n(p)$ when the Impulse Approximation (IA) is valid. In isotropic systems, the scattering in the IA is directly proportional to the longitudinal momentum distribution[1]

$$J_{IA}(Y) = \frac{1}{2\rho\pi^2}\int_{|Y|}^{+\infty} pn(p)dp = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} n(p_x, p_y, Y)dp_x dp_y \qquad (1.1)$$

which is a function of a single scaling variable $Y \equiv (M/Q)(\omega - \omega_r)$, where $M$ is the mass of the scatterer, $Q$ is the momentum transfer, and $\omega_r = Q^2/2M$ is the recoil energy.

However, the experimentally attainable $Q$'s are not large enough to reach the IA limit. Deviations from the IA due to final state scattering by neighboring atoms, known as final state effects, will distort the observed scattering from the IA prediction. Thus, an understanding of deviations from the IA is essential to accurate determinations of $n(p)$.

Liquid helium provides an excellent testing ground for studying FSE in a dense, strongly interacting system for two reasons. First, theoretical calculations of the momentum distribution are available in both the normal liquid[2,3] and superfluid[4] phases. These calculations are believed to be quite accurate, since they agree well with several other measured properties of the liquid. In addition, $n(p)$ in the superfluid exhibits a very sharp feature, the Bose condensate peak, which should be very sensitive to FSE. Comparison of the predicted scattering obtained from the theoretical $n(p)$ using the IA to the experimentally observed scattering can be used to study deviations due to FSE.

## EXPERIMENTAL RESULTS

The scattering from liquid helium was measured at temperatures of 0.35 K and 3.5 K at a density of 0.147 $gm/cm^3$ with the PHOENIX spectrometer at the Intense Pulsed Neutron Source at Argonne National Laboratory using a momentum transfer of 23 $Å^{-1}$ at the recoil peak. The observed scattering is shown in Fig. 1. The empty cell scattering and a small broad component due to secondary scattering from the walls of the cryostat have been subtracted. The scattering, which has been normalized using measurements of low density helium gas, satisfies the first moment sum rule indicating that all the scattering is observed.

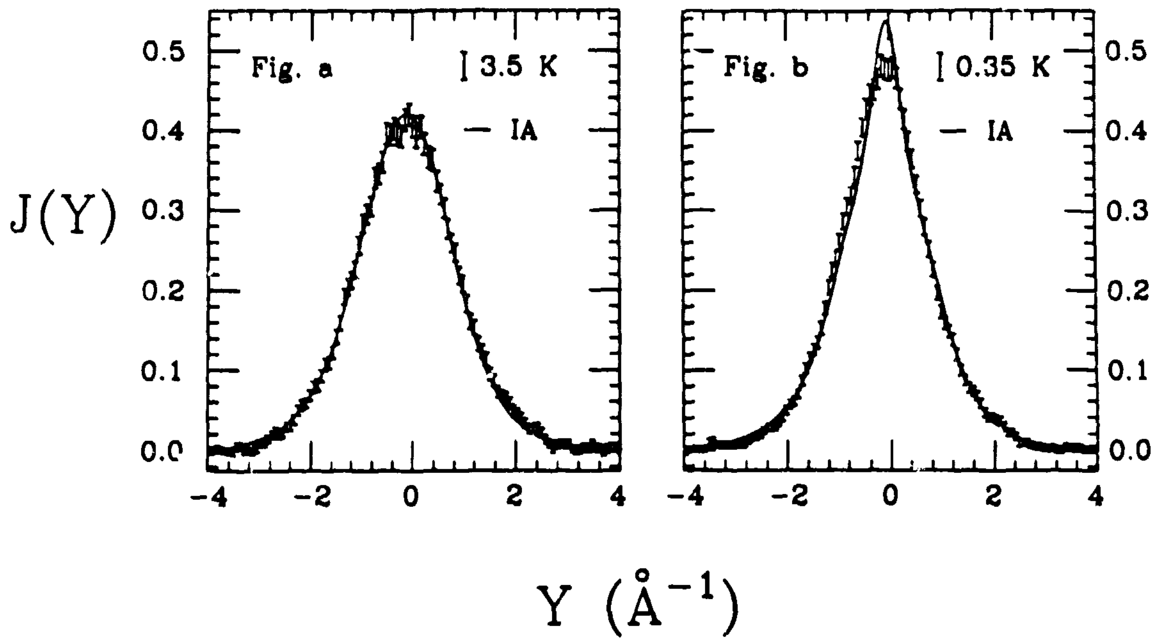


Fig. 1 Observed scattering from liquid $^4$He. a) Normal liquid at T= 3.5 K. The line is the instrumentally broadened IA prediction using the PIMC calculation of $n(p)$. b) Superfluid at T=0.35 K The line is the instrumentally broadened IA prediction using the GFMC calculation of $n(p)$.

The observed scattering exhibits the characteristic features of scattering in the IA. First of all, it is approximately centered at $Y = 0$ and symmetric about $Y = 0$ when instrumental resolution is taken into account. In addition, the width of $J(Y)$ is independent of $Q$ for $Q$'s larger than 15 $Å^{-1}$.[5] However, while the observation of these characteristic features is consistent with the approach to the IA limit, it does not imply that the limit has been reached.[6,7]

To evaluate the applicability of the IA, the observed scattering can be directly compared to the theoretical calculations of $n(p)$. Of course, this approach implicitly assumes that the theoretical momentum distributions accurately describe the true momentum distributions in the liquid. Given the success of these calculations in reproducing many measured properties of the superfluid and normal liquid, we are confident that the momentum distribution is also quite accurate and hence that this method for studying FSE is justified.

The solid line in Fig. 1a is the predicted scattering using the IA and a PIMC calculation of $n(p)$ at T=3.33 K by Ceperley and Pollock. The calculation was carried out at a density of 0.138 gm/cm$^3$, which is slightly lower than the experimental density. The theoretical prediction has been convoluted with the instrumental resolution obtained from a Monte Carlo simulation of the instrument. The overall normalization of both the predicted and observed scattering are independently fixed so that no adjustable parameters have been used.[8] The agreement between the IA prediction and the observed scattering is excellent. Deviations from the IA due to FSE have little effect on the relatively broad and featureless distribution in the normal liquid.

The solid line in Fig. 1b is the predicted scattering using the IA and a GFMC calculation of $n(p)$ at T=0 by Whitlock and Panoff. Large differences between the IA prediction and the observed scattering are obvious. The deviations are largest near $Y = 0$, where the condensate peak occurs. The IA prediction has much more intensity in the peak than observed experimentally, as one would expect from final state smearing of the condensate peak.

Several theoretical calculations[9,10,11] (referred to as broadening theories in this paper) have expressed FSE as a convolution with the IA expression in $Y$. The scattering at finite $Q$ then takes the form

$$J_{FS}(Y) = \int J_{IA}(Y')R(Y' - Y, Q)dY' \tag{2.1}$$

where $J_{FS}$ is the observed scattering including FSE and $R(Y, Q)$ is the final state broadening. The FSE broadening may then be determined by deconvoluting the instrumental broadening and $J_{IA}(Y)$ from the observed scattering.

The superfluid phase, where the deviations from the IA prediction are the largest, provides an excellent opportunity to test this procedure. Fig. 2 shows the results of deconvoluting $J_{IA}(Y)$, obtained from the GFMC calculation of $n(p)$, and the instrumental resolution from the observed scattering in the superfluid. The experimentally determined FSE broadening exhibits a sharp central peak and oscillatory tails that extend to high $|Y|$. While the general features of this curve are accurate, the detailed shape may be affected by the statistical noise in the numerical deconvolution procedure.

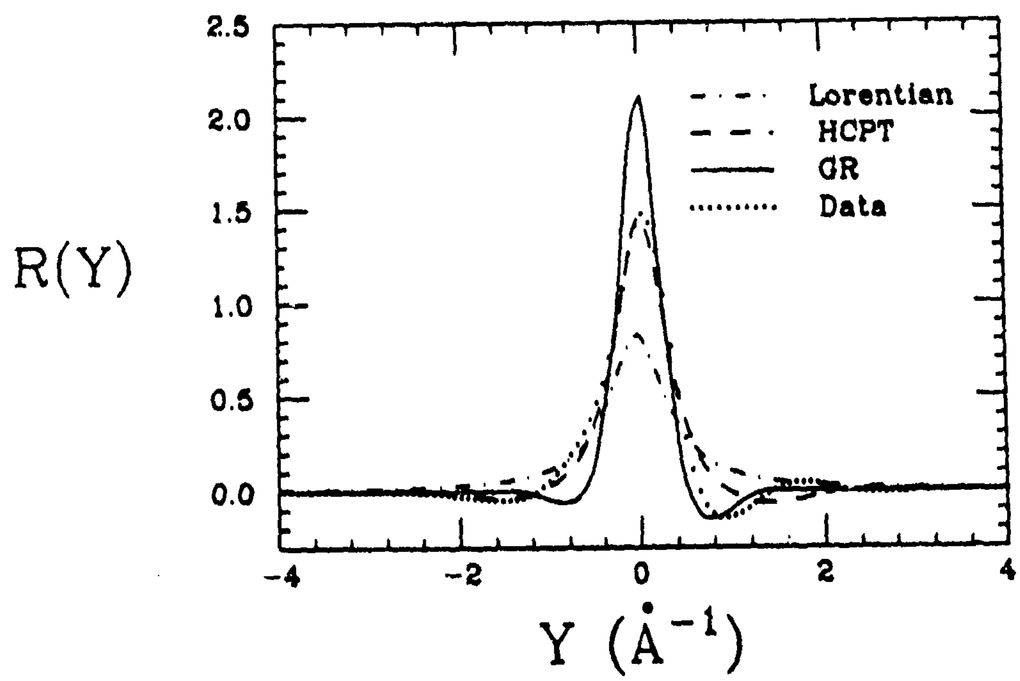


Fig. 2 Comparison of the experimentally determined final state broadening (Data) with theoretical predictions.

There are two noteworthy features in the experimentally determined $R(Y)$. First, the central peak, which is the most prominent feature, is relatively narrow. The full width at half maximum (FWHM) of this peak is 0.67 Å$^{-1}$, narrower than the width expected based on the measured helium-helium scattering cross section. Secondly, $R(Y)$ exhibits oscillatory tails that are both negative and positive. These tails are a natural consequence of the sum rules for incoherent scattering. In particular, the second moment sum rule requires that FSE not change the second moment of the

..., negative tails are required to cancel the contribution of the central peak to the second moment. The negative tails have the important consequence that FSE do not simply broaden the scattering: they move intensity around from one region of $Y$ to another.

In principle, this procedure could be used to determine FSE broadening in the normal liquid. However, due to the statistical accuracy of the data ($\sim 3\%$) and the small effect of FSE, as seen in Fig. 1a, it is not possible to extract a final state broadening function using the same procedure as above. The experimental results require much better statistics before a broadening function can be experimentally determined in the normal liquid.

Another set of theories[12,13,14] (referred to as symmetrization theories here) expresses deviations from the IA as additive corrections to the IA result. In this approach, it is useful to split the corrections to the IA into terms that are symmetric and antisymmetric about the peak center. Then

$$J_{obs}(Y) = J_{IA}(Y) + \Delta J_{Sym}(Y,Q) + \Delta J_{Asym}(Y,Q) \tag{2.2}$$

where $\Delta J_{Sym}$ and $\Delta J_{Asym}$ are the symmetric and antisymmetric corrections due to FSE.

To obtain the corrections to the IA, the theoretical prediction using the IA must be subtracted from the measured scattering after the instrumental broadening has been removed. Rather than deconvolute the instrumental resolution from the data, which is a numerically unstable procedure with noisy data, we will use a model $J_{FS}(Y)$ which is the sum of two Gaussians. The model scattering is broadened by instrumental resolution and compared with the observed scattering, and the model parameters are adjusted to obtain the best agreement.

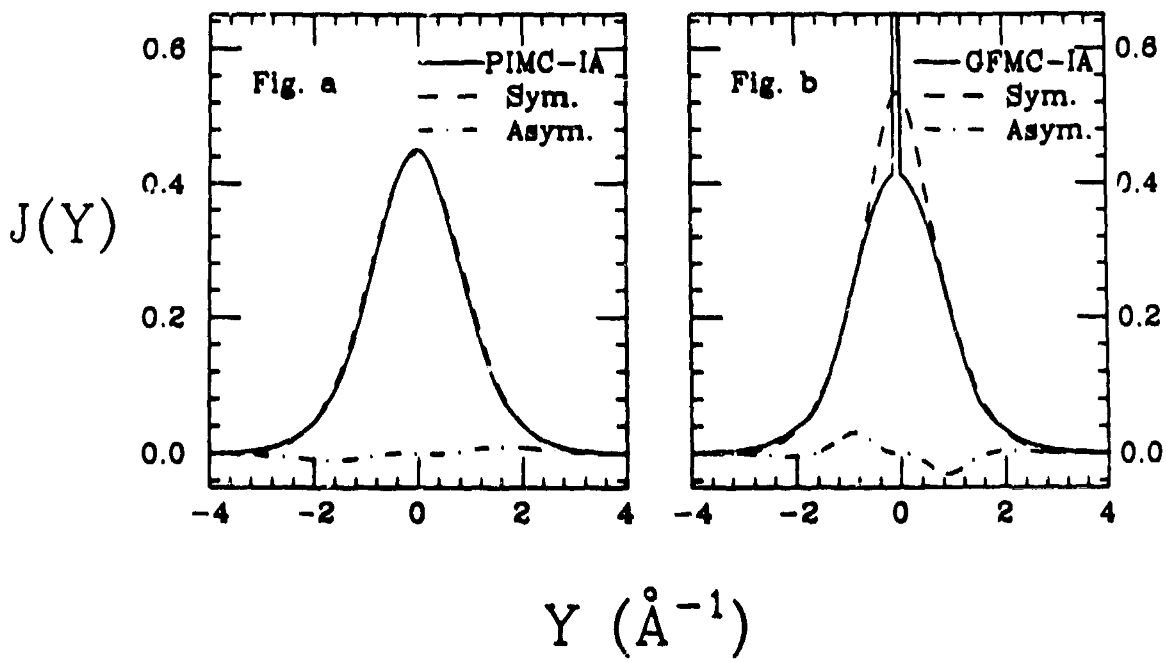


Fig. 3 Comparison of the IA predictions in the normal and superfluid phase with the model $J_{FS}(Y)$ obtained from a fit to the data. The components of $J_{FS}(Y)$ symmetric and antisymmetric about the recoil peak at $Y = 0$ are plotted separately.

The corrections to the IA in the normal liquid, obtained using $n(p)$ from the PIMC calculations of Ceperley, are shown in Fig. 3a. Both the symmetric and antisymmetric corrections are small. The maximum amplitude of the corrections

... % of the total peak amplitude, comparable to the statistical accuracy of the data. The small size of the corrections is not surprising, given the good agreement of the IA prediction and the observed scattering shown in Fig. 1a.

The corrections to the IA in the superfluid, obtained using the $n(p)$ from the GFMC calculations of Whitlock and Panoff, are shown in Fig. 3b. Both the symmetric and antisymmetric correction terms are now much larger than in the normal liquid. The maximum amplitude of the antisymmetric correction is now $\approx$ 20 % of the total peak amplitude, compared to $\approx$ 5 % in the normal liquid. The symmetric correction has a peak amplitude of $\approx$ 25 % of the total peak amplitude. In addition, it contains a negative delta function singularity with 9.2% of the total intensity, which is needed to cancel the condensate delta function in $J_{IA}(Y)$.

## COMPARISONS WITH FINAL STATE EFFECT THEORIES

Theories for FSE can be tested by direct comparison to the observed scattering. The same procedure as used previously will be applied. The theoretical calculations for $n(p)$ are used to obtain the scattering in the IA. The results are then corrected for FSE, using the appropriate theory, and broadened by instrumental resolution. These results may then be compared directly to the observed scattering to evaluate the theories for FSE.

The earliest theory, by Hohenberg and Platzman, predicted a Lorentzian final state broadening. Several other theories have predicted similar behavior. The width of the FS broadening is

$$\Gamma(Q) = \rho\sigma(Q) \tag{3.1}$$

where $\rho$ is the density and $\sigma(Q)$ is the cross section for atom-atom scattering. The Lorentzian broadening for the experimental conditions of this work is shown in Fig. 2. Fig. 4 shows a comparison of the theoretical and experimental results in both the normal and superfluid phases. In both cases the broadening is far larger than observed experimentally. The theoretical results are not in agreement with the experimental observations using a Lorentzian broadening function with the width in (3.1).

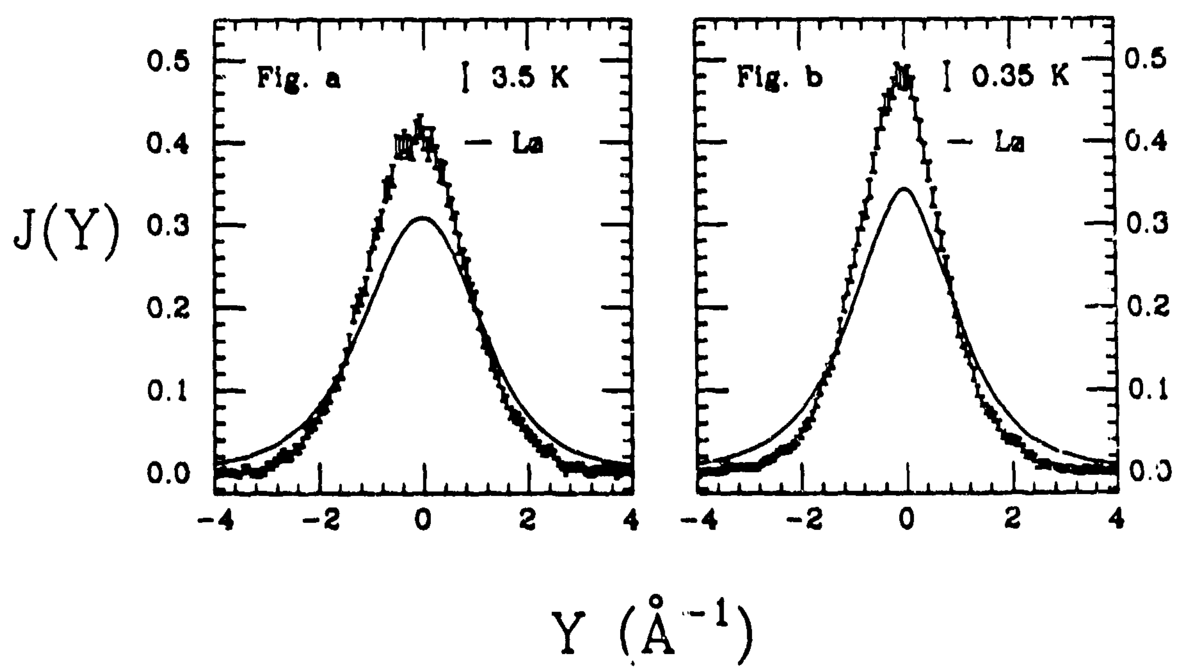


Fig. 4 Comparison of the observed scattering with the theoretical predictions, converted to J(Y) and broadened by instrumental resolution, using a Lorentzian broadening function.

... have obtained a final state broadenig that is not Lorentzian. Instead it contains a narrow central peak and negative tails, as required by the second moment sum rule. The calculated broadening is shown in Fig 2. Fig. 5 shows a comparison of the predicted and observed scattering. The agreement in the normal liquid is excellent. However, in the superfluid phase, the predicted intensity at the peak is too large.

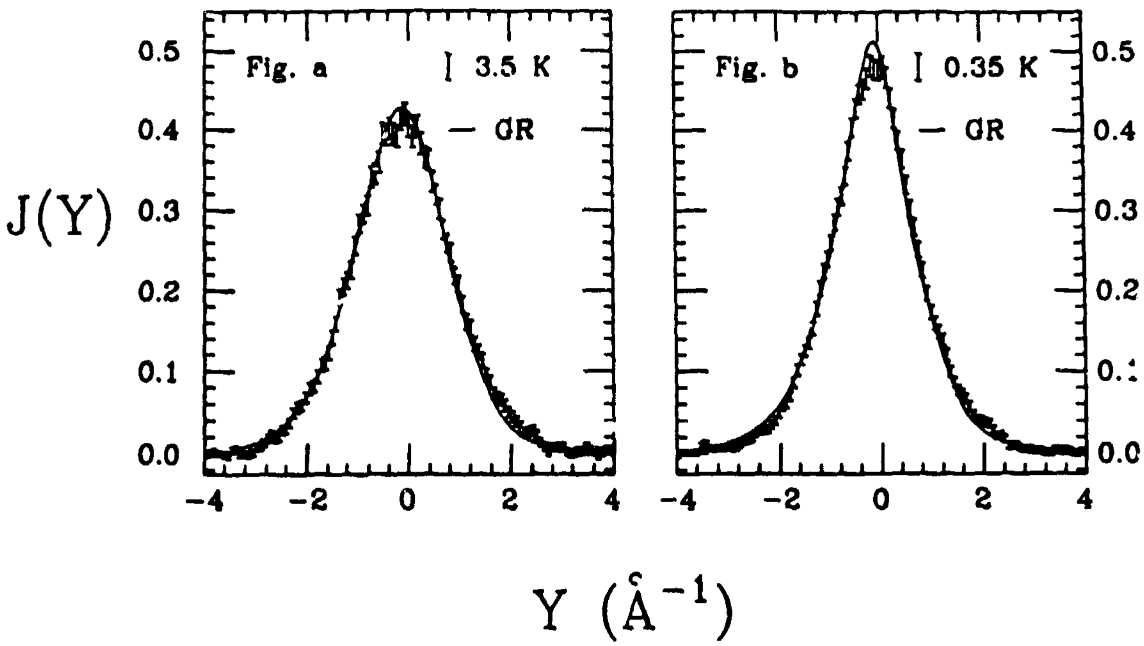


Fig. 5 Comparison of the observed scattering with the theoretical predictions, converted to J(Y) and broadened by instrumental resolution, using the broadening calculated by Gersch and Rodriguez.

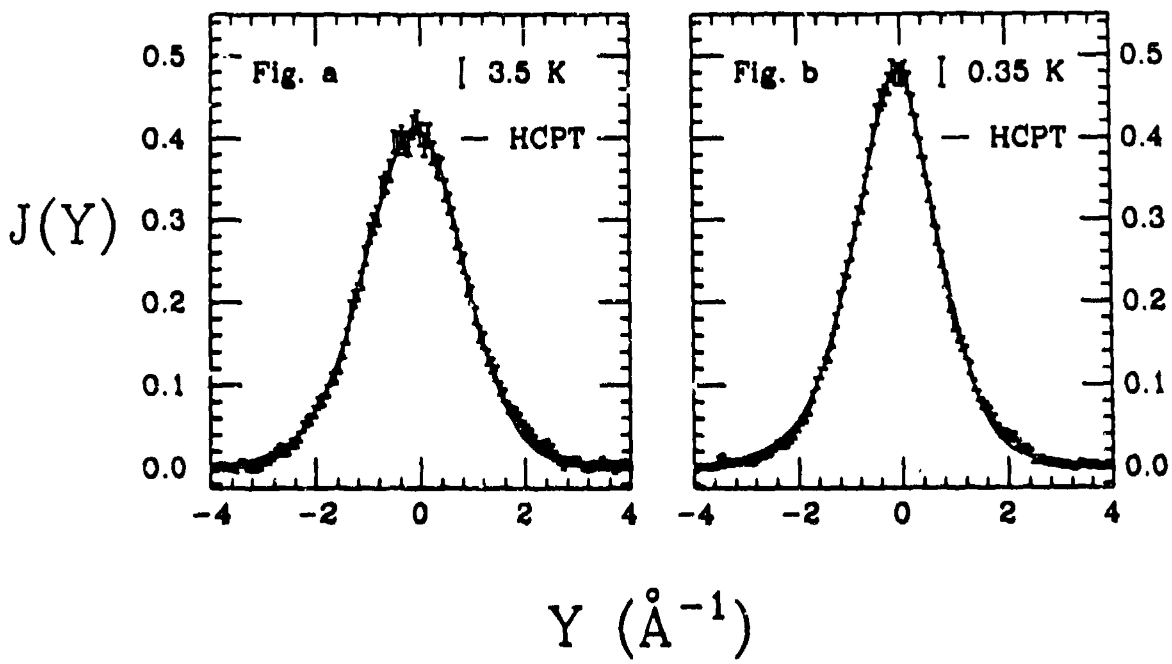


Fig. 6 Comparison of the observed scattering with the theoretical predictions, converted to J(Y) and broadened by instrumental resolution, using the broadening calculated by Silver.

Rodriguez using a method called Hard Core Perturbation Theory (HCPT). The broadening for the experimental conditions used in this measurement is shown in Fig 2. A comparison of the predicted and observed scattering using Silver's theory is shown in Fig. 6. The agreement is excellent in both the superfluid and normal liquid phases.

Symmetrization theories for FSE express differences from the IA as additive corrections to the IA result. These corrections are then split into terms that are either symmetric or antisymmetric about the peak center. The theories estimate the antisymmetric term to be much larger than the symmetric term. If the antisymmetric corrections are dominant, then most of FSE can be removed by simply symmetrizing the data. The removal of the antisymmetric term leaves both the first and second moments of the data unchanged, so this procedure does not violate the second moment sum rule for incoherent scattering.

In the normal liquid, as shown in Fig. 3a, both the symmetric and antisymmetric corrections are small. The symmetrization treatment of FSE corrections does not modify the second moment of the data. Thus, it will have little effect on the broad, nearly gaussian momentum distribution in the normal fluid, and its results will be consistent with the data.

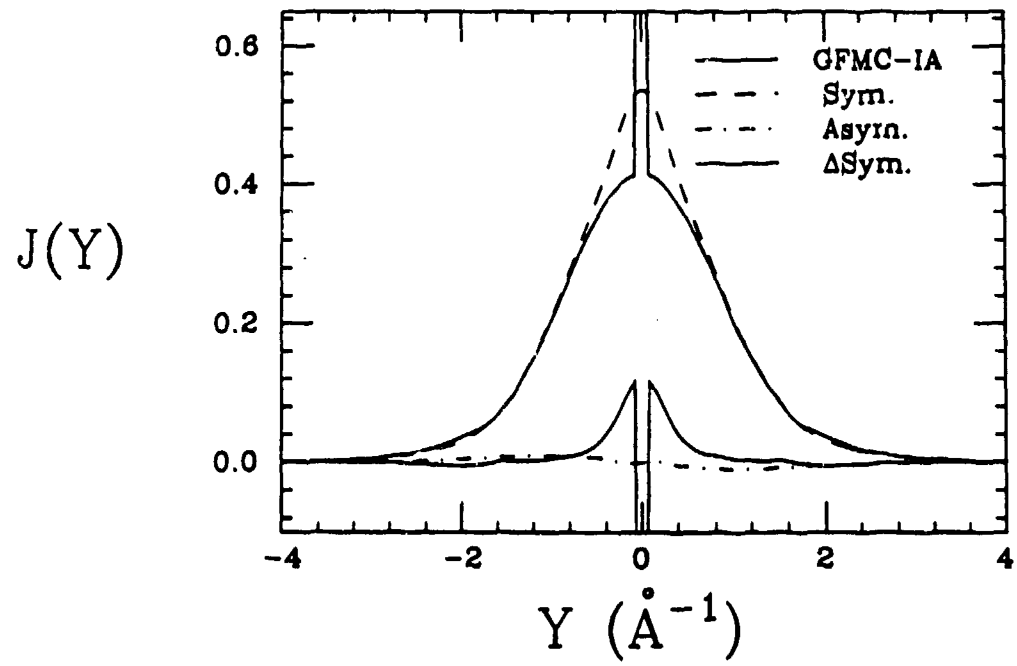


Fig. 7 Symmetric and antisymmetric components of Silver's HCPT prediction for the superfluid scattering versus the IA prediction using the T=0 K GFMC momentum distribution.

In the superfluid, as shown in Fig. 3b, the symmetric and antisymmetric corrections are much larger than in the normal fluid. The symmetric correction consists of a negative delta function singularity with 9.2% of the total intensity superimposed on a positive piece with a peak amplitude of approximately 25% of the total peak amplitude. The negative delta function is required to cancel the condensate delta function that appears in $J_{IA}(Y)$.

The symmetrization theories claim that the IA prediction is reproduced when the FSE broadened momentum distribution is symmetrized. If Silver's HCPT and the symmetrization theories were both correct, then symmetrizing the HCPT prediction should reproduce the IA. In Fig. 7 the IA prediction using the T=0 K GFMC momentum distribution is compared with HCPT and its symmetric and antisymmetric components. Symmetrizing the HCPT prediction does not reproduce the IA. The as shown above, HCPT provides an accurate description of FSE broadening in the superfluid phase, it follows that the symmetrization approach fails.

This figure also shows why the symmetrization procedure fails in the superfluid. The observed scattering contains no feature with a width comparable to the instrumental resolution. Thus, the delta function singularity in $J_{IA}(Y)$ due to the condensate must be removed and replaced with a broadened peak if the IA corrections are expressed as additive terms. The dominant correction to $J_{IA}(Y)$ is then large and symmetric, and it cannot be removed by symmetrizing the data.

## CONCLUSIONS

We have carried out a test of various theories for final state broadening by comparing the observed scattering in the normal and superfluid phases of liquid helium with theoretical predictions for the scattering, using current calculations for the momentum distribution as input. Implicit in our test is the assumption that the theoretical calculations of the momentum distribution are accurate. Our conclusions regarding the FSE theories are valid only to the extent that the theoretical calculations are accurate.

We find that the calculations of Gersch and Rodriguez, Silver, and the symmetrization procedures provide a good description of the FSE for the observed scattering in the normal liquid where $n(p)$ is broad and featureless. The only theories which fail in the normal liquid are those that predict Lorentzian broadening. These theories predict a scattering that is much broader than observed experimentally.

In the superfluid phase, only the calculation of Silver provides an accurate description of the final state broadening. The other models of FSE do not accurately describe the observed scattering in the superfluid phase. Inelastic neutron scattering experiments at other values of $Q$ could test more detailed features of FSE theories.

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