Scaling and deep inelastic neutron scattering from quantum liquids and solids

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A new scaling variable is proposed for investigation of deep inelastic neutron scattering from quantum liquids and solids. The method improves the usual impulse approximation, accounting for a shift of the quasielastic peak with respect to the free recoil energy $\hbar^2q^2/2m$ and for an asymmetric behavior of the wings in the dynamic structure function. The approach is successfully employed to investigate the experimental data in liquid ^{4}He at $q=10$ Å^{-1}.

The occurrence of scaling phenomena in deep-inelastic scattering has been pointed out in several domains of physics as, for example, in neutron scattering from liquids[1] and in elecron scattering from nucleons[2] and nuclei.[3] Though not explicitly mentioned, the concept of scaling has also been employed in the investigation of Compton scattering[4,5] from atoms, molecules, and metals, and of neutron scattering from quantum liquids[6-11] and solids[12,13] where extensive use of the impulse approximation (IA) has been made. In fact, the IA[14] provides the following expression for the dynamic structure function:

$$S^{\mathrm{IA}}(q,\omega)=\int n(\mathbf{p})\delta\left[\omega-\frac{1}{2m}(\mathbf{p}+\mathbf{q})^2+\frac{1}{2m}\mathbf{p}^2\right]d\mathbf{p}\ , \quad (1)$$

and consequently states that the quantity $qS(q,\omega)$ scales[15] in the variable

$$y_0=\frac{m}{q}\left[\omega-\frac{1}{2m}q^2\right] \quad (2)$$

as

$$qS^{\mathrm{IA}}(q,\omega)=2\pi m\int_{|y_0|}^{\infty}pn(p)dp\ . \quad (3)$$

In Eqs. (1)–(3), $n(p)$ is the momentum distribution of the system, and q and ω are the momentum and energy transfers, respectively ($\hbar=1$). In deriving Eq. (3) we have neglected, for the sake of simplicity, possible anisotropies in the momentum distribution. Though the IA can be shown to yield the exact dynamic structure function in the asymptotic limit $q\rightarrow\infty$ and for sufficiently soft potentials,[15,16] it has been pointed out[1,6,7,11,12] that at finite momentum transfer it provides only a semiquantitative description of deep-inelastic neutron scattering in interacting many-body systems, the effects of the interaction being taken into account only through the momentum distribution. Microscopic calculations of $S(q,\omega)$ which take into explicit account the role of the interaction, are now becoming available for liquid[17,18] and solid[19] helium systems at zero temperature. One of the limits of the IA is that it predicts the dynamic structure function $S(q,\omega)$ to be symmetric in the variable $\omega-\omega_R$ [$\omega_R=(1/2m)q^2$ is the free recoil energy] for any value of q. This behavior is contradicted by experiments[1,6,7,11] which show that the peak energy is shifted to the left with respect to ω_R and that the wing at the right of the peak is higher than the one at the left. If one divides the response function into its symmetric and antisymmetric parts with respect to $\omega-\omega_R$,

$$\begin{aligned}S^{(s)}(q,\omega)&=\tfrac{1}{2}[S(q,\omega)+S(q,2\omega_R-\omega)]\ ,\\ S^{(a)}(q,\omega)&=\tfrac{1}{2}[S(q,\omega)-S(q,2\omega_R-\omega)]\ ,\end{aligned} \quad (4)$$

the antisymmetric part has then the typical oscillatory behavior of Fig. 1 where the experimental data[7] for liquid ^{4}He at $T=1.2$ K are reported. The oscillations close to ω_R are a consequence of the shift of the peak, the other two are associated with the asymmetric behavior of the wings. In order to extract the momentum distribution from experiments a symmetrization procedure is commonly employed.[1,9,20] The method essentially makes use of the symmetric part $S^{(s)}(q,\omega)$ of the measured structure function in order to determine $n(p)$ via Eq. (1). In this way one expects to remove first-order corrections in $1/q$ due to the interaction, corrections which are instead present in the antisymmetric part $S^{(a)}(q,\omega)$.

The systematic occurrence of the above deviations with respect to the IA and their independence of the nature of

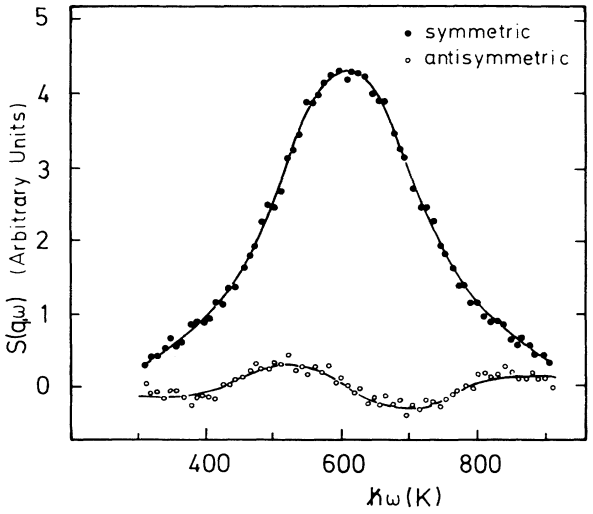

FIG. 1. Experimental values (Ref. 7) for $S^{(s)}(q,\omega)$ and $S^{(a)}(q,\omega)$ [Eq. (4)] in liquid ^{4}He at $T=1.2$ K and $q=10$ Å^{-1}. The full lines are obtained by inserting the momentum $n(p)$ distribution of Ref. 7 into Eq. (7) and taking $\langle K\rangle=14$ K.

the system (liquid, solid), as well as on statistics (^{3}He, ^{4}He), suggest that the shift of the peak and the asymmetry of the tails are a general feature of condensed systems at low temperatures.

The purpose of this paper is to suggest a possible mechanism responsible for such effects, emphasizing the condensed nature of the target. A similar method has been already employed for investigating deep-inelastic electron scattering from nuclei.[21] The IA treats the motion of the atom colliding with the neutron as completely free. In particular, it ignores the fact that in condensed systems at zero temperature the atom occupies a bound state before collision, and also that in the final state the scattered atom interacts with the rest of the system. The drawback of the IA is expected to be particularly significant when large values of p are involved in the integral (1), i.e., in the wings of the structure function. In fact, in this case the IA gives an unphysically large energy to the atom before collision. The simplest way to improve the IA is to replace the energy $p^2/2m$ of the atom before collision with an average binding energy ε and to add an average potential energy V to the kinetic energy $(\mathbf{p}+\mathbf{q})^2/2m$ of the scattered atom. The structure function then becomes

$$S(q,\omega)=\int n(p)\delta\left(\omega-\frac{(\mathbf{p}+\mathbf{q})^2}{2m}-V+\varepsilon\right) .$$

If one requires the counting sum rule $\int S(q,\omega)\omega\, d\omega = q^2/2m$ to be satisfied, the quantity $\varepsilon - V$ is found to coincide with the average kinetic energy per particle $\langle K\rangle = \frac{1}{2}m\int n(p)p^2 d\mathbf{p}$ of the system. The structure function then takes the following form free of adjustable parameters:

$$S(q,\omega)=\int n(p)\delta\left(\omega-\frac{(\mathbf{p}+\mathbf{q})^2}{2m}+\langle K\rangle\right) d\mathbf{p} . \tag{5}$$

Though the two-body force does not appear explicitly in Eq. (5), the effects of the interaction (in particular the binding of the system) play a crucial role in its derivation. In particular, Eq. (5) exhibits significant differences with respect to the structure function of a free gas. Of course only some average effects of the interaction are taken into account in Eq. (5). Explicit final-state interaction effects should be considered for a more detailed description, as required, for example, in the study of the broadening of the momentum condensate in the dynamic structure function of superfluid ^{4}He.[22]

Integration over $\mathbf{p}$ in Eq. (5) yields (an isotropic momentum distribution is also assumed here)

$$qS(q,\omega)=2\pi m\int_{|p_-|}^{p_+} pn(p)dp , \tag{6}$$

where $p_\pm=[2m(\omega+\langle k\rangle)]^{1/2}\pm 1$. Equation (6) shows that the quantity $qS(q,\omega)$ scales in a single variable only for large values of q and ω such that $p_+ \gg |p_-|$ (such a condition is usually well satisfied in deep-inelastic reactions). In this case one can write

$$qS(q,\omega)=2\pi m\int_{|y_1|}^{\infty} pn(p)dp , \tag{7}$$

where

$$y_1=[2m(\omega+\langle K\rangle)]^{1/2}-q \tag{8}$$

is the new scaling variable. One should notice that the scaling function (7) is the same as in the usual IA [Eq. (3)]. It is the scaling variable which differs in the two cases. Some interesting properties of the structure function emerge in the new approach. First of all the peak energy is given by

$$\omega_{\text{peak}}=\frac{1}{2m}q^2-\langle K\rangle , \tag{9}$$

i.e., is shifted to the left with respect to the recoil frequency ω_R by an amount given by the kinetic energy. The observed shifts in liquid ^{4}He (Refs. 6 and 7) ($\sim$10 K) as well as in liquid ^{3}He (Ref. 11) ($\sim$10–20 K) and in solid ^{4}He (Ref. 12) ($\sim$20–30 K) are consistent with the expected values for the kinetic energy of such systems. One should, however, consider Eq. (9) as an estimate of the average peak energy, the present method being unable to predict the observed oscillatory behavior of the shift as a function of q. That the shift of the peak is negative and of the same order of magnitude as the kinetic energy is also confirmed by the theoretical calculations of Ref. 19 for solid ^{4}He and ^{3}He. Another important effect predicted by Eqs. (7) and (8) is the asymmetry of the wings. This effect is entirely due to the fact that the quantity $|y_1|$, differently from $|y_0|$, is not symmetric with respect to $\omega-\omega_R$. The symmetric and antisymmetric parts of $S(q,\omega)$ can be more explicitly evaluated by expanding the scaling variable y_1 in powers of $1/q$ for a fixed value of y_0. Retaining terms up to $1/q$ one finds

$$y_1=y_0+\frac{1}{q}(m\langle K\rangle-\tfrac{1}{2}y_0^2) , \tag{10}$$

$$qS^{(s)}(q,\omega)=2\pi m\int_{|y_0|}^{\infty} pn(p)dp , \tag{11}$$

$$qS^{(a)}(q,\omega)=2\pi m\frac{y_0}{q}n(y_0)(m\langle K\rangle-\tfrac{1}{2}y_0^2) . \tag{12}$$

Equation (12) exhibits the correct q dependence as expected from general arguments.[1] In particular, $y_1\to y_0$ and $qS^{(a)}(q,\omega)\to 0$ when $q\to\infty$ in agreement with the fact that the IA is expected to be asymptotically exact. Equation (12) predicts the zeros of $S^{(a)}(q,\omega)$ to be given by

$$\omega-\omega_R=\pm\frac{q}{m}(2m\langle K\rangle)^{1/2} , \tag{13}$$

independently of the form of $n(p)$ [$\omega=\omega_R$ is also, by definition, a zero of $S^{(a)}(q,\omega)$]. Equations (12) and (13) suggest the possibility of extracting the value of the kinetic energy of the system by looking at the shift between the zeros of $S^{(a)}(q,\omega)$ and the free recoil energy. From the experimental data of Fig. 1 one can extract such a shift with a reasonably good precision, the resulting value for $\langle K\rangle$ being $\sim$14 K, which is a reasonable value for liquid ^{4}He at low temperatures. The present model predicts the above shift to increase linearly with the momentum transfer q. The explicit experimental confirmation of such behavior would be desirable. The correctness of Eq. (13) for giving the zeros of $S^{(a)}$ in the high q limit can be formally proved in the model of Ref. 19 for solid ^{3}He and ^{4}He.[23]

In order to evaluate the dynamic structure function $S(q,\omega)$ through Eqs. (7) and (8) one needs the momen-

tum distribution of the system. By taking the results of Ref. 7 for $n(p)$ and assuming $\langle K\rangle = 14$ K [the above results for $n(p)$ do not allow for an accurate direct estimate of $\langle K\rangle$], we obtain the results of Fig. 1 (full curve). It is worth noticing that the antisymmetric part is well reproduced in the present approach based on the scaling variable y_1. The good agreement for the symmetric part is not surprising. It simply indicates that higher-order corrections in $1/q^2$ in $S^{(s)}(q,\omega)$ [Eq. (11)] are negligible, i.e., that the symmetrization procedure used in Ref. 7 to extract $n(p)$ is highly accurate in this case.

The importance of the antisymmetric part can be more generally discussed using a Gaussian model for the momentum distribution:

$$n(p) = (\tfrac{4}{3}\pi m\langle K\rangle)^{-1/2}\exp\left[-\frac{3}{4}\frac{p^2}{\langle K\rangle m}\right] .$$

One then finds that the ratio between the maximum heights of $S^{(a)}$ and $S^{(s)}$ is given by

$$\frac{S^{(a)}(\max)}{S^{(s)}(\max)} = \frac{1}{q}(2m\langle K\rangle)^{1/2}b^{1/2}\exp(-b) , \qquad (14)$$

with $b = \frac{1}{2}(3+\sqrt{6})$. Prediction (14) agrees with the theoretical results of Ref. 19 for solid ^{3}He and ^{4}He in a very accurate way. In particular, it explains why the IA limit ($S^{(a)}=0$) is reached more rapidly in solid ^{4}He at lower density than at higher density, and more rapidly in ^{3}He than in ^{4}He.

In conclusion I have proposed a new scaling variable for investigating the dynamic structure function in condensed systems at low temperatures. The new approach, which is expected to improve the usual impulse approximation at finite values of momentum transfer, accounts for a symmetric as well as for an antisymmetric component in $S(q,\omega)$ with respect to $\omega-\omega_R$. Clearly the explicit and systematic experimental verification of the new scaling behavior would be highly desirable. In partieular, it would allow for a safer determinaton of the momentum distribution in quantum liquids and solids.

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[1]V. F. Sears, Phys. Rev. B **30**, 44 (1984).
[2]A. Bodek *et al.*, Phys. Rev. D **20**, 1471 (1979).
[3]I. Sick, D. Day, and J. S. McCarty, Phys. Rev. Lett. **45**, 871 (1980).
[4]M. Cooper, Adv. Phys. **20**, 453 (1971).
[5]*Compton Scattering,* edited by B. Williams (McGraw-Hill, New York, 1977).
[6]R. A. Cowley and A. D. B. Woods, Can. J. Phys. **49**, 177 (1971).
[7]P. Martel, E. C. Svensson, A. D. B. Woods, V. F. Sears, and R. A. Cowley, J. Low Temp. Phys. **23**, 285 (1976).
[8]V. F. Sears, E. C. Svensson, P. Martel, and A. D. B. Woods, Phys. Rev. Lett. **49**, 279 (1982).
[9]H. A. Mook, Phys. Rev. Lett. **51**, 1454 (1983).
[10]P. E. Sokol, K. Sköld, D. L. Price, and R. Kleb, Phys. Rev. Lett. **54**, 909 (1985).
[11]H. A. Mook, Phys. Rev. Lett. **55**, 2452 (1985).
[12]V. J. Minkiewicz, T. A. Kitchens, G. Shirane, and E. B. Osgood, Phys. Rev. A **8**, 1513 (1973).
[13]R. O. Hilleke, P. Chaddah, R. O. Simmons, D. L. Price, and S. K. Sinha, Phys. Rev. Lett. **52**, 847 (1984).
[14]P. C. Hohenberg and P. M. Platzman, Phys. Rev. **152**, 198 (1966).
[15]G. B. West, Phys. Rep. **18C**, 263 (1975).
[16]J. J. Weinstein and J. W. Negele, Phys. Rev. Lett. **49**, 1016 (1982).
[17]H. R. Glyde and S. I. Hernadi, Phys. Rev. B **29**, 4926 (1984).
[18]E. Manousakis and V. R. Pandharipande, Phys. Rev. B **33**, 150 (1986).
[19]H. R. Glyde, J. Low Temp. Phys. **59**, 561 (1985).
[20]B. Tanatar, G. C. Lefever, and H. R. Glyde, J. Low Temp. Phys. **62**, 489 (1986).
[21]C. Ciofi degli Atti, Nuovo Cimento **76A**, 330 (1983).
[22]P. M. Platzman and N. Tzoar, Phys. Rev. B **30**, 6397 (1984).
[23]H. Glyde (private communication).