

TITLE THEORY OF NEUTRON SCATTERING EXPERIMENTS ON MOMENTUM DISTRIBUTIONS IN QUANTUM FLUIDS

LA-UR--87-2534

DE87 013169

AUTHOR(S): Richard N. Silver

SUBMITTED TO The 11th International Workshop on Condensed Matter Theories, Oulu, Finland, July 27 to August 1, 1987.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy.

MASTER

Los Alamos Los Alamos National Laboratory Los Alamos, New Mexico 87545

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

THEORY OF NEUTRON SCATTERING EXPERIMENTS ON MOMENTUM DISTRIBUTIONS IN QUANTUM FLUIDS

Richard N. Silver

MS B262, Theoretical Division
Los Alamos Neutron Scattering Center
Los Alamos National Laboratory
Los Alamos, NM 87545

I. INTRODUCTION

Momentum distributions are of fundamental interest to our understanding of the many body physics of quantum solids and fluids. Since the original suggestion by Hohenberg and Platzman,¹ there have been many experiments² with the goal of determining momentum distributions by scattering neutrons at momentum transfer high enough to invoke the impulse approximation (IA). The IA is questionable for helium, because the He-He potential is steeply repulsive at short distances leading to significant final state corrections. These must be understood in order to extract from experiment the parameters of interest, such as the Bose condensate fraction in ⁴He or the Fermi surface discontinuity in ³He. Most theories for final state corrections^{1,3-5,6} have predicted a quasi-Lorentzian broadening of the IA. However, Gersch, et al.⁷ argued, via a complex many-body cumulant derivation, that real space correlations result in a non-Lorentzian final state broadening. A simple quasiclassical theory for this prediction was given by Silver and Reiter,⁸ who expressed the corrections in terms of the radial distribution function, $g(r)$, and the He-He cross action. Until now a fully quantum theory, which included the correct physics for the quantitative correction of experiment, has been lacking.

In this paper, I present the first perturbative derivation of the final state corrections to the impulse approximation for deep inelastic neutron scattering experiments. The final state broadening is found to depend on $g(r)$ and the He-He phase shifts. The theory satisfies the f -sum rule, the ω^2 sum rule ("kinetic energy") valid at high Q , and the ω^3 sum rule. In the structure of the theory, the self-energy terms alone would lead to quasi-Lorentzian broadening. However, these are exactly canceled by a part of the vertex terms which introduce $g(r)$. Numerical results are presented for superfluid ⁴He.

II. MOTIVATION

Let us review the physical picture first discussed by Gersch, et al.⁷ and derived in a quasiclassical approximation by Silver and Reiter.⁸

A neutron scattering from a helium quantum fluid instantaneously imparts a momentum transfer Q and an energy transfer ω to an atom. The impulse approximation (IA) is obtained if Q and ω are large compared to any of the momentum and energy scales characterizing the fluid, so that the helium atom can be assumed to recoil freely. Then $Q S(Q, \omega)$ is a function only of a "scaling" variable, $Y = M(\omega - \hbar Q^2/2M)/\hbar Q$, and it is simply related to the initial momentum distribution $n(p)$ according to

$$Q S_{IA}(Q, \omega) = F_{IA}(Y) = \frac{Q}{\rho} \int \frac{d^3 p}{(2\pi)^3} n(p) \delta\left(\omega - \frac{\hbar Q^2}{2M} - \hbar \frac{\vec{Q} \cdot \vec{p}}{M}\right) \quad (1)$$

This equation has been extensively used in the analysis of experiment.²

However, the He-He potential is steeply repulsive at short distances violating the conditions for the IA. The final state scattering of the He atom by its neighbors should broaden the IA, according to

$$Q S(Q, \omega) = F(Y) = \int_{-\infty}^{\infty} dY' R_{FS}(Y - Y') F_{IA}(Y') \quad (2)$$

$R_{FS}(Y)$ would be a Lorentzian¹ in the simple approximation that the He atom scatters at a constant rate $1/2 \rho v \sigma_{He-He}$ where ρ is density, $v = \hbar Q/M$ is velocity, and σ_{He-He} is the cross section.

In reality, the final state scattering rate is not a constant because the initial positions of the helium atoms are strongly correlated. Figure 1 shows the He-He potential⁹ and the radial distribution¹⁰ function, $g(r)$, for ^4He . The atoms sit in the attractive part of the potential ($r > 2.7 \text{ \AA}$) at some distance from the steeply repulsive core ($r \leq 2.3 \text{ \AA}$) responsible for the final state scattering at high Q . In Wigner's quasiclassical approximation,¹¹ the variable Y is conjugate to the distance which the recoiling atom travels before reaching the core. As there are few collisions at very small collision distance, $R_{FS}(Y)$ should be narrower than the Lorentzian prediction and lack Lorentzian tails.

To obtain this physics in a fully quantum theory, I must retain the full correlations in the ground state, expressed through $g(r)$, in a calculation of the dynamical scattering law, $S(Q, \omega)$, given by

$$S(Q, \omega) = \frac{R_0}{iN} \int_0^{\infty} dt e^{i\omega t - \epsilon t} \langle \hat{\rho}_{-Q}(0) e^{i\hat{H}t/\hbar} \hat{\rho}_Q(0) e^{-i\hat{H}t/\hbar} \rangle \quad (3)$$

Here, $\hat{\rho}_Q(0) = \sum_k \hat{A}_{k+Q}^\dagger \hat{A}_k$ is the density operator, N is the number of particles, $\langle \rangle$ denotes expectation values in the ground state of the full Hamiltonian, \hat{H} , including the interactions responsible for the strongly correlated $g(r)$ and $n(p)$. I do not wish to calculate $g(r)$ and $n(p)$. Rather, I take them as a given property of the ground state $|\psi_0\rangle$ such as obtained by a variational or Monte Carlo calculation, or from a neutron diffraction experiment.

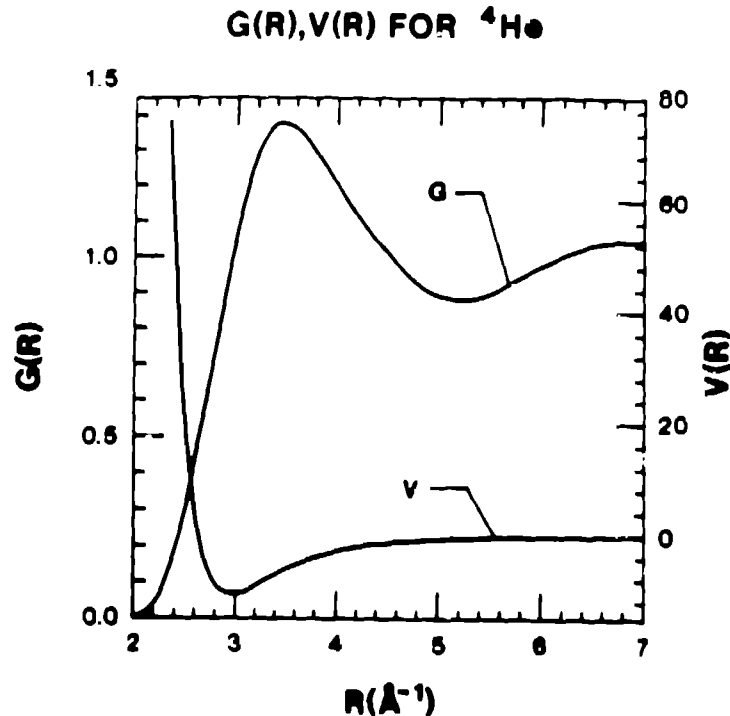


Fig. 1 He-He potential, $V(r)$, and the radial distribution function, $g(r)$, for ^4He at $T = 0^\circ\text{K}$.

If I naively proceed to perturbatively expand only the time dependent part of (3), I find an infinite number of terms which diverge as inverse powers of $\omega - \mathbf{A}\mathbf{Q}^2/2M + i\epsilon$. A method for infinite order resummation is required. The Kubo formula for the frequency dependent electrical conductivity in a metal, $\sigma(\omega)$, has a form similar to Eq. (3). A similar problem occurs in which perturbation expansion results in an infinite number of divergent terms in inverse powers of $\omega + i\epsilon$. One solution of this problem is to use Liouville perturbation theory and a diagonal projection operator method to resum all the singular terms.¹² I adopt a similar procedure to evaluate $S(\mathbf{Q},\omega)$, except that I use an off-diagonal projection operator appropriate for $\mathbf{Q} = 0$. As is true for the perturbative derivation of Boltzmann equation answers for the resistivity starting from the Kubo formula, I find that vertex terms must be retained and these introduce the correlations, $g(r)$.

In terms of Feynman diagrams, the perturbative expansion of Eq. (3) should yield the Dyson equation shown in Fig. 2. I assume that \mathbf{Q} is sufficiently high that the dynamics of low momentum holes, created by \hat{a}_k and represented by \leftarrow , occurs over a much longer time scale than the dynamics of high momentum particles, created by \hat{a}^\dagger_{k+q} and represented by \rightarrow . The wiggly lines represent T-matrices. So the dynamics of holes can be ignored, but their instantaneous spatial correlations (defined by $g(r,t)$ for $t = 0$) are important. If only the bare and self energy terms in Fig. 2 are included, the result would be quasi-Lorentzian broadening of the IA.³ The vertex term in Fig. 2 includes a hole four point function, represented by \boxtimes , which is related to $g(r) - 1$. Inclusion of the vertex term yields a non-Lorentzian final state broadening of the IA. A precise meaning to the diagrams in Fig. 2 will be given in Secs. III and IV.

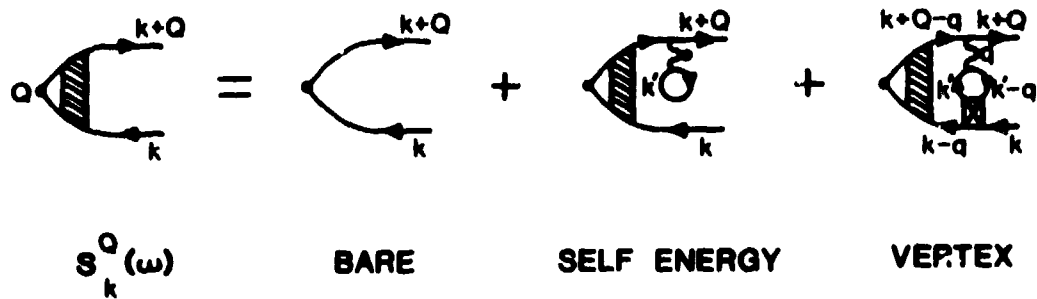


Fig. 2 Diagrammatic representation of the Dyson equation for deep inelastic neutron scattering.

III. HARD CORE PERTURBATION THEORY FOR DYNAMICS

In this section, I present a general framework for the Liouville perturbative expansion of $S(Q, \omega)$ in terms off-diagonal projection operator methods and ground state expectation values of products of creation and annihilation operators. In the following section I specialize to the particular case of "deep inelastic neutron scattering" (DINS) at high Q .

I define a "superoperator" as an operator \hat{S} which acts on the ordinary operator to its right, say \hat{O} , to create a new ordinary operator \hat{O}' , according to $\hat{S}\hat{O} = \hat{O}'$. For example the Liouville superoperator \hat{L} is defined by

$$\hat{L}\hat{O} = -i[\hat{H}, \hat{O}] \quad (4)$$

Here \hat{O} denotes an ordinary operator constructed out of sums of products of scalars and creation and annihilation operators, and \hat{S} denotes a superoperator. If \hat{H} can be written as the sum of kinetic, \hat{K} , and potential, \hat{V} , terms, then similarly $\hat{L} = \hat{K} + \hat{V}$.

Consider then the quantity which occurs in $S(Q, \omega)$, Eq. (3)

$$\hat{S}^Q(\omega) = \int_0^\infty dt e^{i\omega t - \epsilon t} e^{i\hat{H}t} \hat{p}_Q(0) e^{-i\hat{H}t} \quad (5)$$

In terms of superoperators

$$\hat{S}^Q(\omega) = \frac{i\hat{A}}{\hbar\omega - \hat{L}} \hat{p}_Q(0) \quad (6)$$

Eq. (6) can be expanded as a Dyson equation

$$\hat{S}^Q(\omega) = \frac{i\hat{A}}{\hbar\omega - \hat{K} + i\epsilon} \hat{p}_Q(0) + \frac{1}{\hbar\omega - \hat{K} + i\epsilon} \hat{V} \hat{S}^Q(\omega) \quad (7)$$

Since $\hat{K} \hat{A}^+_{k+Q} \hat{A}_k = (\epsilon_{k+Q} - \epsilon_k) \hat{A}^+_{k+Q} \hat{A}_k$, the singular terms in the expansion of (7) as inverse powers of $\omega + i\epsilon - \hbar Q^2/2M$ occur as $(\hbar\omega^+ - \hat{K})^{-1}$ operates on terms of the form $\hat{A}^+_{k+Q} \hat{A}_k$.

In general, $\hat{S}^Q(\omega)$ has the form of an infinite summation of terms consisting of a scalar times products of creation and annihilation operators. Following the treatment¹² of the singular terms in the Kubo formula developed by Argyres and Sigel, I seek a projection superoperator $\hat{\Delta}$ which projects out only those components of an operator, \hat{O} , which create single particle excitations of momentum Q out of the ground state, i.e.

$$\tilde{\Delta}\hat{O} = \sum_k o_k \hat{a}_{k+Q}^+ \hat{a}_k \quad (8)$$

Argyres and Sigel¹² used a diagonal projection superoperator, $Q = 0$, whereas I use an off-diagonal one. $\tilde{\Delta}$ must also satisfy $\tilde{\Delta}\tilde{\Delta} = \tilde{\Delta}$ and $\tilde{\Delta}\hat{a}_{k+Q}^+ \hat{a}_k = \hat{a}_{k+Q}^+ \hat{a}_k$.

Defining $\tilde{\Delta}' = 1 - \tilde{\Delta}$, straightforward manipulations then yield from the Dyson equation (7) for $\hat{S}^Q(\omega)$

$$\tilde{\Delta}\hat{S}^Q(\omega) = \frac{i\hbar}{\hbar\omega^+ - K} \tilde{p}_Q(0) + \frac{1}{\hbar\omega^+ - K} \tilde{\Delta}\hat{T}\tilde{\Delta}\hat{S}^Q(\omega) \quad (9)$$

where the \hat{T} superoperator is

$$\tilde{\Delta}\hat{T}\tilde{\Delta} = \tilde{\Delta}\tilde{V}\tilde{\Delta} + \tilde{\Delta}\tilde{V}\tilde{\Delta}' \frac{1}{\hbar\omega^+ - K - \tilde{\Delta}'\tilde{V}\tilde{\Delta}'} \tilde{\Delta}'\tilde{V}\tilde{\Delta} \quad (10)$$

Note that (10) is the superoperator analogue of the Hamiltonian \hat{T} matrix equation.

A two body approximation would be to replace $\tilde{\Delta}\hat{T}$ by

$$\tilde{\Delta}\hat{O} = -(\tilde{\Delta}\hat{T}, \hat{O}) \quad (11)$$

where the two body \hat{T} matrix operator is

$$\hat{T} = \frac{1}{2\Omega} \sum_{k_1, k_2, Q} T_{k_1, k_2, Q} \hat{a}_{k_1+Q}^+ \hat{a}_{k_2-Q}^+ \hat{a}_{k_2} \hat{a}_{k_1} \quad (12)$$

Here $T_{k_1, k_2, Q}$ are the scalar components of the \hat{T} -matrix, which can be expressed in terms of the phase shifts and scattering angles when ω is on-energy-shell. Note that exactly this two-body approximation¹² is used in the perturbative derivation of the resistivity starting from the Kubo formula.

I claim the following is an explicit construction of the projection superoperator required

$$\tilde{\Delta}\hat{O} = \sum_k \frac{\hat{a}_{k+Q}^+ \hat{a}_k \langle (\hat{a}_{k+Q}^+ \hat{a}_k)^+ \cdot \hat{O} \rangle}{n_k - n_{k+Q}} \quad (13)$$

Here (A, B) is a commutator, $n_k = \langle \hat{a}_k^+ \hat{a}_k \rangle$, and $\langle \rangle$ denotes ground state average. Remarkably, the same formula works for Bosons and Fermions.

Within the two-body \hat{T} -matrix approximation, I find that Eqs. (3), (9) and (13) constitute a closed system of equations for $\hat{S}(Q, \omega)$. These depend on properties of the ground state through the n_k and through a four-point function

$$\Phi(k_1, k_2, Q) = \langle \hat{a}_{k_1+Q}^+ \hat{a}_{k_2-Q}^+ \hat{a}_{k_2} \hat{a}_{k_1} \rangle \quad (14)$$

Usually I do not have complete information on $\Phi(k_1, k_2, Q)$. I do know its symmetry properties such as $\Phi(k_1, k_2, Q) = \Phi(k_1, k_2, K)$ where $K = k_2 - Q - k_1$. I also know a sum rule

$$\frac{1}{N} \sum_{k_1, k_2} \Phi(k_1, k_2, Q) = N \delta_{Q=0} + \rho \int d^d r e^{iQ \cdot r} (g(r) - 1) \quad (15)$$

which follows from the definition of $S(Q)$. Here, $g(r)$ is the radial distribution function and $\rho = N/\Omega$ is the density. As we shall see, the first term on the right hand side gives rise to self energy terms in the Dyson equations and the second term to vertex terms. Note that the -1 component of the second term exactly cancels the first term.

IV. $S(Q, \omega)$ AT HIGH Q

I now specialize to the problem of deep inelastic neutron scattering (DINS),¹³ which is the behavior of $S(Q, \omega)$ for very high Q . For clarity, I restrict the calculation to ^4He . I will use the concept of high, capital "Q", and low, small "q", momenta to select the important terms at high Q . To define "high" and "low" momenta operationally, a high momentum Q is where to an excellent approximation $nQ \approx 0$ and $\rho \int d^3r e^{iQ \cdot r} (g(r) - 1) \approx 0$ (or $\Delta_Q |\psi_0\rangle \approx 0$). That is high momenta greatly exceed the typical momenta characterizing the condensed phase.

At high Q , I expect that two-body collisions dominate the final state broadening, so that the approximation Eq. (11) is valid. I also expect that the $T_{k_1 k_2 Q}$ can be taken to be the free particle T-matrix because the nq are negligible at high Q . A tedious, but straightforward, expansion of Eqs. (9), (11)-(13) would then yield a complicated set of equations for the components S_k^Q of $\tilde{\Delta} \hat{S}^Q(\omega)$ defined by

$$\tilde{\Delta} \hat{S}^Q(\omega) = \sum_k S_k^Q a_{k+Q}^+ a_k \quad (16)$$

At high Q , I find the following simplifications:

- 1) The projection operator can be reduced to

$$\tilde{\Delta} \hat{O} = \sum'_k \frac{1}{n_k} \left\{ \hat{a}_{k+Q}^+ \hat{a}_k \langle \hat{a}_{k+Q}^+ \hat{a}_{k+Q} \hat{O} \rangle + \hat{a}_k^+ \hat{a}_{k-Q} \langle \hat{O} \hat{a}_{k-Q}^+ \hat{a}_k \rangle \right\} \quad (17)$$

where the prime on the summation means it is restricted to low momenta.

- 2) Terms generated of the form $\hat{a}_k^+ \hat{a}_{k-Q}$ always have negligible coefficients $\Phi(k_1, k_2, Q)$, and so the second term in (17) can be dropped.
- 3) Terms generated from $\hat{T} \hat{a}_k$ are negligible compared with terms generated from $\hat{T} \hat{a}_{k+Q}$, because the corresponding \hat{T} matrices are larger for high momenta due to the steeply repulsive He potential.
- 4) At high Q , the forward and backward scattering Born symmetrized T-matrix

$$T_{k-Q+Q, k-Q}^{sym} = T_{k-Q+Q, k-Q} + T_{k-Q+Q, k-Q} \quad (18)$$

is to a good approximation a function only of Q and q , i.e.

$$\lim_{\text{high } Q} T_{k-Q+Q, k-Q}^{sym} = \bar{T}(Q, q) \quad (19)$$

- 5) I can take $\bar{T}(Q, q)$ to be on-energy-shell since I am interested in $\hbar\omega$ very close to the recoil energy $\hbar^2 Q^2 / 2M$. (I may wish to consider off-energy-shell $\bar{T}(Q, q)$ for smaller Q , which would introduce an asymmetry weighted toward high ω . This could also be important in the problem of electron scattering in nuclear physics.)

Following this line of reasoning, I arrive at a relatively simple equation for the S_k^Q

$$S_k^Q(\omega) = \frac{1}{\hbar\omega - \epsilon_{k+Q} + i\epsilon} \left[i\hbar + \frac{1}{\Omega n_k} \sum_q S_{k-q}^Q(\omega) \bar{T}(Q, q) \sum_{k'} \Phi(k-q, k', q) \right] \quad (20)$$

Consider first the limit of a non-interacting system where $g(r) \rightarrow 1$. Then

$$\lim_{g(r) \rightarrow 1} \frac{1}{n_k} \sum_{k'} \Phi(k-q, k', q) = \delta_{q=0} N \quad (21)$$

would satisfy the sum rule, Eq. (15), and would be the correct non-interacting result. Then (20) is readily solved to yield

$$\lim_{g(r) \rightarrow 1} S_k^Q(\omega) = \frac{1}{\hbar\omega - \epsilon_{k+Q} - \rho \bar{T}(Q, 0)} \quad (22)$$

This is the usual self-energy corrected propagator for a high Q particle in terms of the forward scattering T-matrix. This result would yield quasi-Lorentzian final state broadening of the impulse approximation. (Going off-energy-shell would introduce some asymmetry toward the high ω side of the recoil peak³).

However, $g(r)$ is very different from 1. While I don't exactly know $n^{-1} \sum_k \Phi(k-q, k', q)$, I do know the n_k weighted average of it from the sum rule, Eq. (15). Therefore, I approximate it by its average

$$\frac{1}{n_k} \sum_{k'} \Phi(k-q, k', q) = N\delta_{q=0} + \rho \int d^3r e^{iQr} (g(r) - 1) \quad (23)$$

This will lead to a convolution form of the final state broadening, Eq. (2). When Eq. (23) is substituted into Eq. (20) there are three terms on the right hand side. These terms may be represented by the Feynman diagrams shown in Fig. 2. A solution of Eqs. (20) and (23) can be obtained as follows.

$S_k^Q(\omega)$ is a function only of k_{\parallel} , where parallel (\parallel) is defined with respect to the direction of Q. Then one can sum over q_{\perp} . Define

$$\bar{T}(q_{\parallel}) = \frac{-1}{\Omega^{2D}} \sum_{q_{\perp}} \bar{T}(Q, q) \Phi(q) \frac{M}{\hbar^2 Q} \quad (24)$$

$$I(k_{\parallel}) = \frac{\hbar^2 Q}{M} S_{k_{\parallel}}^Q(\omega) \quad (25)$$

and

$$\Phi(q) = \rho \int d^3r e^{iQr} g(r) \quad (26)$$

Using the scaling variable,¹³ $Y = M(\omega - \hbar Q^2/2M)/\hbar Q$, I obtain

$$(Y - k_{\parallel}) I(k_{\parallel}) = i\hbar + \frac{1}{\Omega^{1/2}} \sum_{q_{\parallel}} I(k_{\parallel} - q_{\parallel}) \bar{T}(q_{\parallel}) \quad (27)$$

The second term of (27) has the form of a convolution, and so the equations can be solved by Fourier transform from momentum space to real space

$$S_{k_1}^Q = \frac{M}{\hbar Q} \int_0^\infty dx e^{ik_1 x} \exp \left\{ i \int_0^x dx' (Y + \Gamma(x')) \right\} \quad (28)$$

where $\Gamma(x)$ is the Fourier transform of $\bar{\Gamma}(q_\perp)$, Eq. (24).

I use semiclassical methods,¹⁴ which are certainly accurate at high Q , to solve for $\Gamma(x)$. I start with the standard expression for T in terms of phase shifts.

$$\bar{\Gamma}(Q, q) = - \frac{4\pi\hbar^2}{\mu Q} \sum_{\ell \text{ even}} (2\ell + 1) e^{2i\delta_\ell} - 1 P_\ell(\cos\theta) \quad (29)$$

At high Q , a large number of ℓ contribute to (29). I can therefore replace the sum by an integral using the Poisson summation formula. The scattering angle, $\theta \approx 2q_\perp/Q$, is small. I can therefore use the large ℓ /small angle representation of Legendre polynomials in terms of Bessel functions

$$P_\ell(\cos\theta) \approx J_0((\ell + 1/2)\theta) = \frac{1}{2\pi} \int_0^{2\pi} \exp \left[i \left(\ell + \frac{1}{2} \right) \frac{2}{Q} \vec{q}_\perp \cdot \vec{n}(\phi) \right] d\phi \quad (30)$$

where $\vec{n}(\phi)$ is a unit vector perpendicular to Q . The summation over q_\perp in (24) simply yields a δ -function involving r_\perp in Eq. (23). I replace the angular momentum ℓ by the impact parameter, $b = (\ell + 1/2)2/Q$. Then $|r_\perp| = b$. I evaluate the phase shifts, $\delta(b)$, using the JWKB approximation.

V. RESULTS FOR DEEP INELASTIC NEUTRON SCATTERING

Following the steps outlined in Sec. IV yields the following final results for final state broadening function as defined in Eq. (2)

$$R_{FS}(Y) = \frac{1}{\pi} \text{Re} \int_0^\infty dx \exp \left\{ i \int_0^x dx' (Y + \Gamma(x')) \right\} \quad (31)$$

where

$$\Gamma(x) = \frac{2\pi\rho}{i} \int_0^\infty b db f_b g(\sqrt{x^2 + b^2}) \quad (32)$$

$$f_b = e^{2i\delta(b)} - 1 + \sum_{M=0} e^{2i\delta(b) + i \frac{M\pi Q}{2} b} \quad (33)$$

$\Gamma(\infty)$ is related by a constant to the He-He T-matrix. Only the $M = -1$ term is significant in the summation in Eq. (33), and it leads to the hard sphere glory oscillations of the He-He cross section. I will refer to Eq. (31) as the "hard core perturbation theory" result (HCPT).

The final results, Eqs. (31)-(33), meet all the requirements for a quantum theory discussed by Silver and Reiter.⁸ Comparing the present results with the quasiclassical theory (QC), I find that the mathematical form from HCPT is remarkably similar. However, in the present theory: 1) forward diffractive scattering is properly taken into account, so that the second term produces glory oscillations (absent in QC) and the large x scattering rate is $1/2\rho v 2\pi r_\perp^2$ ($2 \times$ QC); 2)

the db integrals now involve the phase shifts (rather than the "effective" hard sphere radius in QC), so that steeply repulsive potentials can also be handled; 3) the argument of $g(r)$ is simpler, which allows HCPT to satisfy the ω^2 and ω^3 sum rules¹⁵ for much smaller Q (not true in QC for $Q < 20 \text{ \AA}^{-1}$), and which eliminates the strong dependence on the detailed form of $g(r)$ obtained in the QC theory; 4) the integral in the argument of the exponential extends to x (it was $x/2$ in QC); 5) there is a shift in the peak position due to the real part of $\Gamma(x)$ (absent in QC). I have no explanation for the differences between these two theories.

The HCPT results also differ quantitatively from the work of Gersch, et al.⁷ while they agree regarding the importance of spatial correlations. The decoupling approximation is different, HCPT expresses the results in terms of $g(r)$ where Ref. 7 does not, HCPT properly handles the forward diffractive scattering where Ref. 7 does not, etc.

The HCPT results can be derived by an alternate procedure in which I approximate the Hamiltonian to retain only the high momenta and short distance (i.e. r such that $V(r) \sim O(\hbar^2 Q^2/2M)$) components in the dynamics. The static expectation values are evaluated in a ground state determined from the low momenta and long range parts of the Hamiltonian. This was, in fact, the original route to Eqs. (31)-(33).

Results similar to (31)-(33) can be derived for Fermion systems (e.g. ^3He), except that the summation in (33) must be changed to account for the different statistics.

The final state broadening, Eq. (31), has been evaluated numerically for superfluid ^4He . Figure 3 compares the HCPT resolution function to a

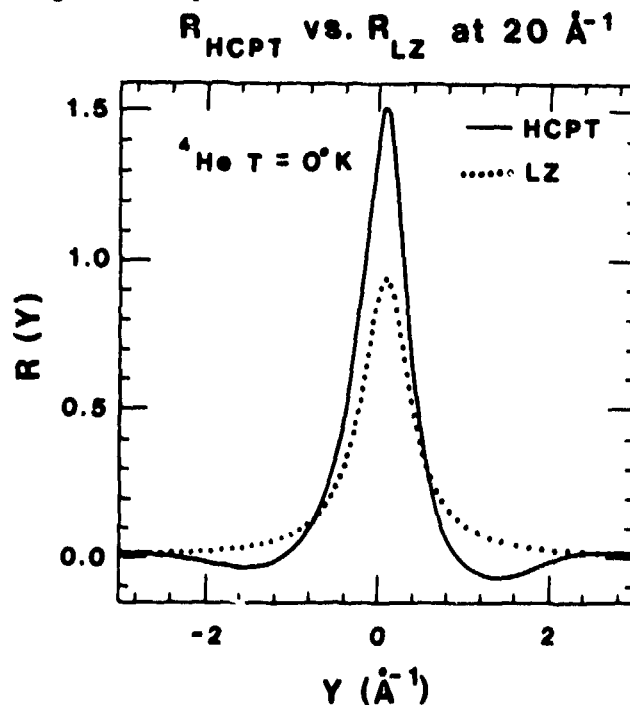


Fig. 3 Final state resolution functions, $R(Y)$, calculated for ^4He at $Q = 20 \text{ \AA}^{-1}$ in the present theory (HCPT) and in the quasi-Lorentzian approximation (LZ).

quasi-Lorentzian (LZ) obtained by taking $g(r) \rightarrow 1$ in Eq. (32). The $R_{\text{HCPT}}(\gamma)$ has a narrower FWHM, a zero second moment satisfying the kinetic energy (ω^2) sum rule, and no high frequency wings.

Figure 4 shows calculations of $QS(Q, \omega)$ for the HCPT, LZ, and IA models using a theoretical momentum distribution calculated by Lam, et al.,¹⁶ which has an 11.9% Bose condensate fraction. For HCPT, the linewidth of the non-condensed atoms is comparable to the IA, but the Bose condensate peak is not clearly resolved. The LZ lineshape is much wider than the HCPT and the IA, and the glory oscillations (not shown) are much larger in LZ than in HCPT. It is remarkable that $QS(Q, \omega)$ turned out to be positive in this calculation as required, even though $R_{\text{HCPT}}(\gamma)$ is both positive and negative. This required a close relationship between $g(r)$ and $n(p)$.

Figure 5 shows the change in $QS(Q, \omega)$ between 20 \AA^{-1} and 200 \AA^{-1} . The Bose condensate peak only slightly sharpens at 200 \AA^{-1} , but it is still not clearly resolved. The approach to the IA is very slow for He (logarithmic in Q), and the IA is never reached for a hard sphere potential no matter how high the Q . Final state corrections are important at any experimentally feasible Q .

Detailed numerical predictions for ^4He , ^3He and the hard sphere Bose liquid will be presented elsewhere.¹⁷

The convolution form for the final state broadening, Eq. (2), can fail for a variety of reasons: the k -dependence of the left hand side of Eq. (23) may be significant; Q may not be high enough to justify the on-energy-shell approximation for the T-matrix, etc. A detailed discussion of the corrections to Eqs. (2) and (31) at

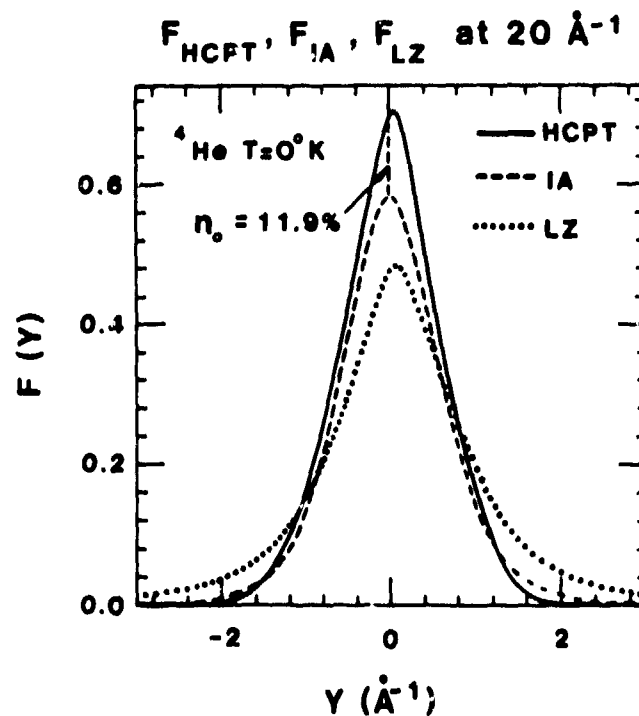


Fig. 4 Calculations of $QS(Q, \omega)$ in the present theory (HCPT), quasi-Lorentzian (LZ), and the impulse approximation (IA) for ^4He at $Q = 20 \text{ \AA}^{-1}$.

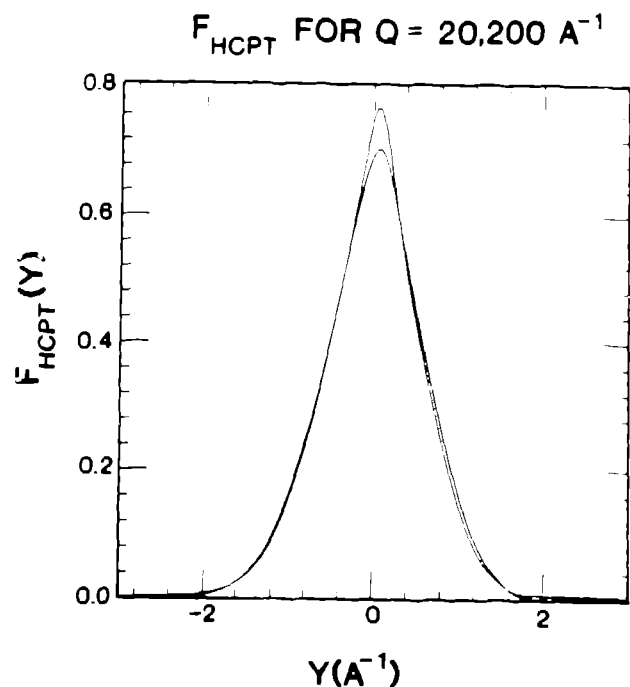


Fig. 5. Calculations of $QS(Q, \omega)$ in the present theory (HCPT) for ${}^4\text{He}$ at $Q = 20 \text{ \AA}^{-1}$ and $Q = 200 \text{ \AA}^{-1}$.

lower Q is beyond the scope of this article, although the Q achieved in present generation experiments may not be high enough to apply the Eqs. (2) and (31) blindly.

VI. CONCLUSION

The hard core perturbation theory of deep inelastic neutron scattering experiments qualitatively confirms the earlier many-body cumulant theory of Gersch, et al.⁷ and the quasiclassical theory of Silver and Reiter.⁸ The quantitative predictions and the structure of the theory are new. I have shown how vertex corrections give rise to a non-Lorentzian, zero second moment lineshape for final state corrections.

The good news for experimentalists is that, at high enough Q , the final state broadening takes the form of a convolution and is smaller than the Lorentzian broadening theories would predict. The bad news is that neither the Bose condensate peak in ${}^4\text{He}$, nor the Fermi surface discontinuity in ${}^3\text{He}$, will be clearly resolved in any feasible DINS experiment. However, provided the final state theory is known and instrumental corrections understood, a deconvolution procedure (such as maximum entropy) might be feasible to extract the singular structures and other features of momentum distributions. There must now be a detailed effort to reanalyze momentum distribution experiment on quantum solids and fluids.

For theorists, it is truly remarkable that a projection superoperator method, originally designed to solve transport problems in the limit of $Q = 0$, can be extended to solve scattering problems at very high Q . This suggests that the

method may be applicable to a wide variety of problems involving the calculation of dynamics, $S(Q, \omega)$, from a knowledge of static correlations, $S(Q)$. An immediate application will be to momentum distribution experiments in nuclear and particle physics, such as electron nucleus scattering.

ACKNOWLEDGMENTS

Special thanks to J. W. Clark for his advice during the course of this project. I also thank K. Bedell, G. Reiter, and P. Sokol for many helpful discussions. This work was supported by the Office of Basic Energy Sciences of the U.S. Dept. of Energy.

REFERENCES

1. P. C. Hohenberg, P. M. Platzman, *Phys. Rev.* **152**, 198 (1966).
2. For reviews, see E. C. Svensson, *Proceedings of the 1984 Workshop on High Energy Excitations in Condensed Matter*, LA-10227, p. 456; P. Sokol in *Proceedings of the 1986 Banff Conference on Quantum Liquids and Solids*, *Can. Journ. Physics* 1987. H. R. Glyde, E. C. Svensson, Chapter 13 in *Neutron Scattering in Condensed Matter Research*, Ed. K. Sköld and D. L. Price, to be published by Academic Press.
3. P. M. Platzman, N. Tzoar, *Phys. Rev. B* **30**, 6397 (1984).
4. T. R. Kirkpatrick, *Phys. Rev. B* **30**, 1266 (1984).
5. G. Reiter, R. Becher, *Phys. Rev. B* **32**, 4492 (1985).
6. For other approaches see J. J. Weinstein, J. W. Negele, *Phys. Rev. Letters* **49**, 1016 (1982) and V. F. Sears, *Phys. Rev. B* **30**, 44 (1984).
7. H. A. Gersch, L. J. Rodriguez, *Phys. Rev.* **A8**, 905 (1973); L. J. Rodriguez, H. A. Gersch, H. A. Mook, *ibid.*, **9**, 2085 (1974).
8. R. N. Silver, G. Reiter, *Phys. Rev. B* **1**, **35**, 3647 (1987).
9. R. Feltgen, H. Kirst, K. A. Kohler, H. Pauly, F. Torello, *J. Chem. Phys.* **76** (5), 2360 (1982).
10. E. C. Svensson, V. F. Sears, A. D. Woods, P. Martel, *Phys. Rev. B* **21**, 3638 (1980).
11. G. Reiter, R. N. Silver, *Phys. Rev. Letters* **54**, 1047 (1985).
12. P. N. Argyres, J. L. Sigel, *Phys. Rev. Letters* **31**, 1397 (1973); *Phys. Rev. B* **9**, 3197 (1974).
13. See G. B. West, *Phys. Reports* **18**, 263 (1975).
14. See, e.g., M. V. Berry and K. E. Mount, *Reports on Progress in Physics*, **35**, 315 (1972); R. K. B. Helbing, *Journal of Chemical Physics*, **50**, 493 (1969).
15. See Appendix A. in E. Feenberg, *Theory of Quantum Fluids*, (Academic Press, New York, 1969).
16. P. M. Lam, J. W. Clark, M. L. Ristig, *Phys. Rev. B* **16**, 222 (1977).
17. R. N. Silver, to be published.