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Theory of deep inelastic neutron scattering on quantum fluids

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The line shape for high-momentum-transfer neutron scattering experiments on quantum fluids is derived by a novel perturbative method which includes the effect of the spatial correlations in the ground state. The final-state broadening of the impulse approximation is shown to be non-Lorentzian, to have a zero second moment, and to be significant for all feasible experiments. There are important implications for the goal of measuring momentum distributions. Numerical results are presented for ^{4}He.

Momentum distributions are fundamental to our understanding of quantum fluids and solids, nuclei, and even elementary particles. There have been many calculations of the momentum distribution n_k by a wide variety of many-body methods.[1] There is also a long history of experiments[2] which attempt to measure n_k by "deep inelastic" scattering at momentum transfers Q, which are high relative to collective behavior. Such experiments presume that the impulse approximation (IA) can be applied at sufficiently high Q. The IA would predict a simple relation between the scattering law $S(Q,\omega)$ and n_k. However, in helium fluids and in nuclei the potentials are steeply repulsive at short distances resulting in significant broadening of the IA due to final-state interactions. Hohenberg and Platzman[3] predicted a Lorentzian broadening of the IA with width proportional to the scattering rate for a high-Q particle. Then, Gersch, and co-workers[4] predicted that spatial correlations, as given by the radial distribution function $g(r)$, result in a non-Lorentzian broadening. Nevertheless, the subsequent theories[5] either ignored $g(r)$ or concluded that $g(r)$ was not important, and they usually predicted quasi-Lorentzian broadening. Experimentalists have also failed to apply the results of Gersch *et al.* to their data analysis. A correct theory for final-state effects is critical to the reliable extraction of n_k from experiment, and it is especially urgent in view of the new generation of momentum distribution experiments on quantum fluids at pulsed neutron sources and on nuclei at electron accelerators.[6]

The goal of this Rapid Communication is to clarify the theory of deep inelastic neutron scattering (DINS) experiments by providing the first perturbative derivation of the final-state broadening which includes the spatial correlations. I introduce dynamical "hard-core perturbation theory" (HCPT) methods which are generally applicable to strongly correlated systems. I show that predictions of quasi-Lorentzian broadening can result from the improper neglect of vertex terms. Relatively simple results for the broadening are derived which depend on the He-He phase shifts and $g(r)$.

The broadening of the IA for $S(Q,\omega)$ at high Q can take the form

$$QS(Q,\omega)\equiv F(Y)=\int_{-\infty}^{\infty}dY'R_{FS}(Y-Y')F_{\mathrm{IA}}(Y') \ . \quad (1)$$

Here, $Y\equiv M(\omega-\hbar Q^2/2M)/\hbar Q$ is the scaling variable[7] and $F_{\mathrm{IA}}(Y)$ is the IA prediction for $QS(Q,\omega)$. Silver and Reiter[5] suggested a quasiclassical model for the broadening, $R_{FS}(Y)$. Before a neutron strikes a He atom, its initial position is in the attractive part of the He-He potential due to its neighbors. After a neutron imparts a high momentum Q, the atom recoils on almost a straight line for some distance until it is scattered by the steeply repulsive core of the potential on a neighboring atom. $R_{FS}(Y)$ is the Fourier transform of the probability for no core collisions as a function of recoil distance. $R_{FS}(Y)$ should have no large Y components (i.e., no Lorentzian wings) due to the absence of collisions at short distances.

In a fully quantum theory, the spatial correlations of the strongly interacting ground state are critical to the calculation of

$$S(Q,\omega)=\frac{1}{\pi N}\langle\hat{S}^Q(\omega)\hat{\rho}_{-Q}(0)\rangle \quad (2)$$

at high Q for ^{4}He, where

$$\hat{S}^Q(\omega)\equiv\int_0^{\infty}dt\,e^{i\omega t-\epsilon t}e^{i\hat{H}t/\hbar}\hat{\rho}_Q(0)e^{-i\hat{H}t/\hbar} \ . \quad (3)$$

Here, the angular brackets denote the ground-state expectation value, $\hat{\rho}_Q(0)=\sum_k\hat{a}^{\dagger}_{k+Q}\hat{a}_k$, and N is the number of particles. A naive expansion of Eq. (3) results in an infinite number of terms which diverge as inverse powers of $\omega-\hbar Q^2/2M+i\epsilon$. This series is analogous to the divergences as inverse powers of $\omega+i\epsilon$ of the perturbative expansion of the Kubo formula for the frequency-dependent conductivity in a metal $\sigma(\omega)$. The Boltzmann equation result for the resistivity may be derived from the Kubo formula by using Liouville perturbation theory and a diagonal projection "superoperator" to resum all the singular terms.[8] In the following, I show that an analogous procedure can be adopted for $S(Q,\omega)$, except that I need an off-diagonal projection superoperator for $Q\neq 0$.

An operator $\hat{O}$ is a sum of products of scalars with creation and annihilation operators. A "superoperator" $\tilde{S}$ acts on an operator on its right to create a new operator $\hat{O}'$ according to $\tilde{S}\hat{O}=\hat{O}'$. For example, the Liouville superoperator $\tilde{L}$ is defined by $\tilde{L}\hat{O}\equiv-[\hat{H},\hat{O}]$. The Liouville perturbative expansion of $\hat{S}^Q(\omega)$, Eq. (3), is given by the

Dyson equation

$$\hat{S}^Q(\omega)=\frac{1}{\hbar\omega-\tilde{K}+i\epsilon}[i\hbar\hat{\rho}_Q(0)+\tilde{V}\hat{S}^Q(\omega)] \ , \quad (4)$$

where $\tilde{K}$ is the kinetic and $\tilde{V}$ the potential part of $\tilde{L}$. The singular terms in inverse powers of $\omega-\hbar Q^2/2M+i\epsilon$ occur as $(\hbar\omega-\tilde{K}+i\epsilon)^{-1}$ acts on terms in $\hat{S}^Q(\omega)$ of the form $\hat{a}^\dagger_{k+Q}\hat{a}_k$. I define a particle-hole projection superoperator $\tilde{\Delta}$ such that

$$\tilde{\Delta}\hat{S}^Q(\omega)=\sum_k S^Q_k(\omega)\hat{a}^\dagger_{k+Q}\hat{a}_k \ , \quad (5)$$

where $S^Q_k(\omega)$ are scalar components of $\hat{S}^Q(\omega)$. $\tilde{\Delta}$ must also satisfy $\tilde{\Delta}\tilde{\Delta}=\tilde{\Delta}$ and $\tilde{\Delta}\hat{a}^\dagger_{k+Q}\hat{a}_k=\hat{a}^\dagger_{k+Q}\hat{a}_k$. The explicit construction is

$$\tilde{\Delta}\hat{O}\equiv\sum_k\frac{\hat{a}^\dagger_{k+Q}\hat{a}_k\langle[(\hat{a}^\dagger_{k+Q}\hat{a}_k)^\dagger,\hat{O}]\rangle}{n_k-n_{k+Q}} \ . \quad (6)$$

Here $[A,B]$ is a commutator and $n_k=\langle\hat{a}^\dagger_k\hat{a}_k\rangle$. Defining $\tilde{\Delta}'\equiv 1-\tilde{\Delta}$, straightforward manipulation yields

$$\tilde{\Delta}\hat{S}^Q(\omega)=\frac{1}{\hbar\omega-\tilde{K}+i\epsilon}[i\hbar\hat{\rho}_Q(0)+\tilde{\Delta}\tilde{T}\tilde{\Delta}\tilde{\Delta}\hat{S}^Q(\omega)] \ , \quad (7)$$

where

$$\tilde{T}\equiv\tilde{V}+\tilde{V}\tilde{\Delta}'\frac{1}{\hbar\omega+i\epsilon-\tilde{K}-\tilde{\Delta}'\tilde{V}\tilde{\Delta}'}\tilde{\Delta}'\tilde{V} \ . \quad (8)$$

Note that (8) is the superoperator analogue of the Hamiltonian $\hat{T}$-matrix equation. So far, this reordering of the perturbation expansion has been exact.

Now, I assume that two-body collisions dominate the final-state scattering at high Q, so that it is safe to make a two-body approximation, $\tilde{T}\hat{O}\simeq-[\hat{T}_2,\hat{O}]$, such that

$$\hat{T}_2=\frac{1}{2\Omega}\sum_{k_1k_2Q}T_{k_1k_2Q}\hat{a}^\dagger_{k_1+Q}\hat{a}^\dagger_{k_2-Q}\hat{a}_{k_2}\hat{a}_{k_1} \quad (9)$$

in terms of the free particle $T_{k_1k_2Q}$. Then Eqs. (6), (7), and (9) constitute a closed system for the $S^Q_k(\omega)$ defined in Eq. (5) in terms of the n_k and the expectation value of the two-particle density matrix

$$\Phi(k_1,k_2,Q)\equiv\langle\hat{a}^\dagger_{k_1+Q}\hat{a}^\dagger_{k_2-Q}\hat{a}_{k_2}\hat{a}_{k_1}\rangle \quad (10)$$

which satisfies a sum rule

$$\frac{1}{N}\sum_{k_1k_2}\Phi(k_1,k_2,Q)=N\delta_{Q=0}+\rho\int d^3r\,e^{iQr}[g(r)-1] \ , \quad (11)$$

where $\rho\equiv N/\Omega$. All the terms in the Dyson equation for $S^Q_k(\omega)$ involve a product of a $T_{k_1,k_2,Q}$ and a $\Phi(k_1,k_2,Q)$, such that the steeply repulsive core of the potential (large Q) is screened by the ground-state correlations. The "small parameter" of this perturbation expansion is $T_2\Phi$, and it is not T or V.

For the DINS problem, I use the concept of "high" and "low" momenta to select the important terms in the Dyson equation for $S^Q_k(\omega)$ at high Q. Operationally, a high momentum, capital Q, satisfies $n_Q\simeq 0$ and $\rho\int d^3r\,e^{iQr}[g(r)-1]\simeq 0$, whereas a low momentum, small q, does not. To be important, a term must have a high momentum in the arguments of T to sample the steeply repulsive core, and it must have no high momenta in the arguments of Φ to have nonzero expectation value in the ground state. Then,

$$S^Q_k(\omega)=\frac{1}{\hbar\omega-\epsilon_{k-Q}+\epsilon_k+i\epsilon}\left(i\hbar+\frac{1}{\Omega n_k}\sum_q S^Q_{k-q}(\omega)\sum_{k'}T^{\mathrm{sym}}_{k+Q-q,k',q}\Phi(k-q,k',q)\right) \quad (12)$$

where T^{sym} is the forward and backward symmetrized T matrix. I approximate $n_k^{-1}\sum_{k'}\Phi(k-q,k',q)$ by its n_k-weighted average from the sum rule, i.e., the right-hand side of Eq. (11). I obtain three terms on the right-hand side of (12) corresponding to the "bare," "self-energy," and "vertex" terms shown in Fig. 1. The bare term alone produces the IA. Adding the self-energy term produces quasi-Lorentzian broadening of the IA. The vertex term introduces the important spatial correlations, $g(r)-1$, resulting in a non-Lorentzian broadening.

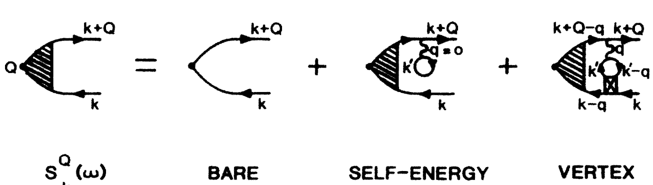

FIG. 1. Diagrammatic representation of the Dyson equation, Eq. (12), for deep inelastic neutron scattering. Here, right arrow denotes a particle line, left arrow a hole line, wiggly line a T matrix, and □ a four-point function in the ground state related by a sum rule to $g(r)-1$.

Equation (12) is solved by Fourier transform to real space, since S^Q_k depends only on the $k_\parallel$ component and the vertex term has the form of a momentum-space convolution. I approximate the T matrix by its on-energy-shell behavior, which can be accurately evaluated at high Q using standard semiclassical methods.[9] Details will be presented elsewhere.

The final HCPT result for $R_{FS}(Y)$ is

$$R_{FS}(Y)=\frac{1}{\pi}\mathrm{Re}\int_0^\infty dx\exp\left(i\int_0^x dx'[Y+\Gamma(x')]\right) \ , \quad (13)$$

$$\Gamma(x)=\frac{2\pi\rho}{i}\int_0^\infty db\,df_b\,g(\sqrt{x^2+b^2}) \ , \quad (14)$$

$$f_b=e^{2i\delta(b)}-1+\exp\left[2i\delta(b)-\frac{i\pi Q}{2}b\right] \ . \quad (15)$$

$\Gamma(\infty)$ is related by a constant to the He-He T matrix expressed in terms of the Jeffreys-Wentzel-Kramers-Brillouin (JWKB) phase shift $\delta(b)$ for impact parameter b. The third term in Eq. (15) is due to Bose statistics, and it leads to the hard-sphere glory oscillations of the He-He cross section.

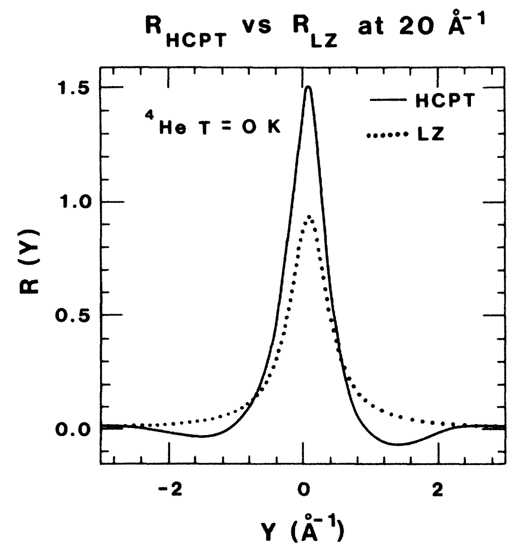

FIG. 2. Final-state broadening function, $R(Y)$, calculated for He at $Q=20$ Å^{-1} in the present theory (HCPT) and in the quasi-Lorentzian (LZ) approximation obtained by taking $g(r)\to 1$.

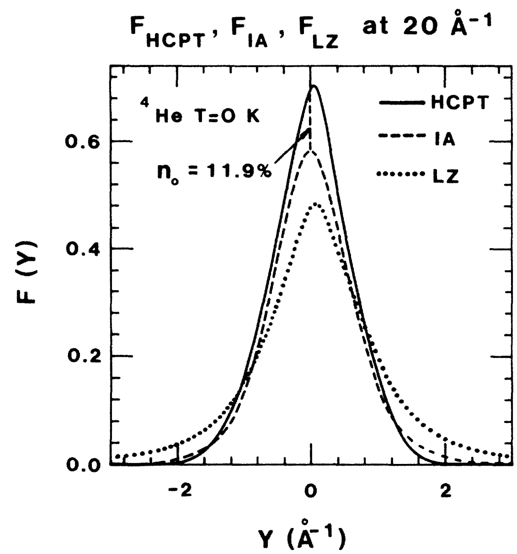

FIG. 3. Calculations of $QS(Q,\omega)\equiv F(Y)$ in the present theory (HCPT), quasi-Lorentzian (LZ), and the impulse approximation (IA) for ^{4}He at $Q=20$ Å^{-1}.

$R_{FS}(Y)$, Eq. (13), has been numerically evaluated for ^{4}He at $T=0$ K and $Q=20$ Å^{-1} using experimental $g(r)$ (Ref. 10) and $V(r)$.[11] Figure 2 compares HCPT to a quasi-Lorentzian (LZ) obtained by taking $g(r)\to 1$ in Eq. (14). $R_{\rm HCPT}(Y)$ has a narrower full width at half maximum (FWHM), a zero second moment, and no high-frequency wings. Figure 3 shows calculations of $F(Y)$ for the HCPT, LZ, and IA models using a theoretical momentum distribution by Lam *et al.*[12] which has an 11.9% Bose condensate fraction. The linewidth of the noncondensed atoms is comparable in HCPT and IA, while it is much larger in LZ. The Bose condensate peak is not clearly resolved in either HCPT or LZ. The high $|Y|$ components are suppressed in HCPT compared with the IA. Calculations as a function of Q (not shown) reveal a logarithmic decrease with Q of the width of $R_{FS}(Y)$. The IA is never reached for the hard-sphere Bose liquid at high Q even though Y scaling is obtained. Hard-sphere glory oscillations in the width of $F(Y)$ in the LZ theory are suppressed in HCPT for $Q>10$ Å^{-1}.

This theory captures the leading behavior at high Q of the final-state broadening. It satisfies the f sum rule to $O(Q^{-3})$, the ω^3 sum rule to $O(Q^{-1})$, and the ω^2 (kinetic energy) sum rule at high Q to $O(Q^{-2})$.[13] It shifts the motivation for pushing DINS experiments to higher Q from "approaching the impulse approximation" to "approaching a limit where final-state corrections are understood." The new pulsed neutron source data are at much higher Q than reactor data, but comparison is complicated by the effect of the instrument resolution function. Such HCPT predictions as an absence of high $|Y|$ (Lorentzian) wings around the recoil peak, negligible broadening of the noncondensed atom distribution, an asymmetric line shape, and significant broadening of the Bose condensate peak appear to be confirmed by experiment,[2] although careful study is needed.

HCPT provides a straightforward path for the systematic improvement of these calculations. Inclusion of the off-energy-shell behavior of the T matrix would lead to a more complex $R_{FS}(Y)$ which is weighted toward the high Y side of the recoil peak. The question of a significant k dependence of $n_k^{-1}\sum_{k'}\Phi(k-q,k',q)$ could be tested by a correlated basis function evaluation of Φ. Recent Green's-function Monte Carlo results[1] yield more reliable n_k.

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