Theory of deep inelastic neutron scattering: Hard-core perturbation theory

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(Received 11 January 1988; revised manuscript received 15 March 1988)

Details are presented of a new many-body theory for deep inelastic neutron scattering (DINS) experiments to measure momentum distributions in quantum fluids and solids. The high-momentum and energy-transfer scattering law in helium is shown to be a convolution of the impulse approximation with a final-state broadening function which depends on the scattering phase shifts and the radial distribution function. The predicted broadening satisfies approximate Y scaling, is neither Lorentzian nor Gaussian, and obeys the f, ω^2, and ω^3 sum rules. The derivation uses a combination of Liouville perturbation theory, projection superoperators, and semiclassical methods which I term "hard-core perturbation theory." A review is presented of the predictions of prior theories for DINS experiments in relation to the present work. A subsequent paper will present massive numerical predictions and a discussion of DINS experiments on superfluid ^{4}He.

I. INTRODUCTION

This paper is the first of two to present details of a recent theory[1] for deep inelastic neutron scattering (DINS) experiments in quantum solids and fluids. The present paper focuses on the many-body formalism including extensive comparisons with prior work. A subsequent paper[2] is aimed at experimentalists and presents detailed numerical predictions for DINS experiments on superfluid ^{4}He. Variations of this theory are also applicable to DINS experiments on many other systems where momentum distributions are of current interest. These include normal ^{3}He, solid ^{4}He and ^{3}He, ^{4}He-^{3}He mixtures, solid H_2, hydrogen in metals, H_2 intercalated in graphite, hydrogen bonds, etc. The theory may also be adapted to nuclear physics problems such as quasielastic inclusive electron-nucleus scattering. Since completing this work, there has been spectacular experimental confirmation of this theory for superfluid ^{4}He, to be published elsewhere.[3]

DINS experiments involve neutron scattering at momentum and energy transfers which are very high compared with collective behavior. The goal is to measure the single-particle momentum distribution, n_k. This would critically test our fundamental concepts of quantum many-body systems such as the existence of a Bose condensate in superfluid ^{4}He, a Fermi-surface discontinuity in normal ^{3}He fluid, and the absence of these singularities in the solid phase. It would test a variety of many-body calculations by techniques such as correlated basis functions,[4] Green's-function Monte Carlo,[5] and path-integral Monte Carlo.[6] Momentum distributions are also important in nuclear[7] and particle[8] physics, where they are studied by analogous deep inelastic experiments.

The theoretical understanding of the scattering law, $S(Q,\omega)$, at high Q and ω is critical to the extraction of n_k from the experiment. Hohenberg and Platzman[9] suggested in 1966 that the impulse approximation (IA) could be applied to calculate $S(Q,\omega)$ for neutron scattering at sufficiently high-momentum transfers. The IA assumes that the potential energy due to neighboring particles can be ignored at sufficiently high kinetic energies. It predicts a simple relation between $S(Q,\omega)$ and n_k. The center of the scattering would be at $\omega=Q^2/2M$, and the peak width would be proportional to Q times the width of the momentum distribution. More generally, the IA predicts that $QS(Q,\omega)$ is a symmetric function of a single "scaling" variable, $Y\equiv M(\omega-Q^2/2M)/Q$. This result has been termed "Y scaling,"[10] and it has been an especially important concept in quasielastic inclusive electron-nucleus scattering.[11]

However, in helium and in nuclei the potentials are steeply repulsive at short distances resulting in significant broadening of the IA due to the scattering of the recoiling particle from neighboring particles. This broadening is a "final-state effect" (FSE), which is the subject of this paper. If we denote the IA result for $QS(Q,\omega)/M$ by $F_{\mathrm{IA}}(Y)$, then in several theories the actual scattering law $QS(Q,\omega)/M\equiv F(Y)$ is a convolution of a "FSE broadening function," $R_{\mathrm{FS}}(Y)$, with $F_{\mathrm{IA}}(Y)$. The theories for FSE can be characterized in the "asymptotic limit" which may be accurately defined as the broadening of the IA in the limit of a hard-core short-range potential and infinite Q. The longer-range part of the potential is assumed to be finite affecting ground-state properties such as n_k and $g(r)$, but not affecting the FSE. In the asymptotic limit the FSE should satisfy Y scaling, which implies that $R_{\mathrm{FS}}(Y)$ will be independent of Q. The broadening must satisfy the sum rules on $S(Q,\omega)$. In particular, the ω^2 ("kinetic energy") sum rule[12] requires that the second moment of $R_{\mathrm{FS}}(Y)$ should be zero.

The true He-He potential is exponentially repulsive at short distances, i.e., $\overline{V}(r)\propto e^{-ar}$, or equivalently the He-He cross section decreases as $\ln Q$.[13,14] To apply the asymptotic limit to real experiments on helium at finite Q, one must use an "effective" Q-dependent hard-core radius which will decrease as $\ln Q$ at high Q. This radius can be defined as the classical turning point of the potential for a particle of momentum Q, and it will be discussed in more detail in Sec. IV. The width of $R_{\mathrm{FS}}(Y)$ will decrease as $\ln Q$ at high Q reflecting the behavior of the He-He cross section.

There have been many theories of FSE in the twenty-two years since Hohenberg and Platzman's[9] paper. While a detailed discussion can be found in the original papers, I will briefly mention those predictions which are relevant to the present work. Several theories have nontrivial asymptotic limits; Hohenberg and Platzman[9] proposed that $R_{\mathrm{FS}}(Y)$ in helium was Lorentzian [asymptotic limit of $R_{\mathrm{FS}}(Y) \propto Y^{-2}$ at high $|Y|$] with width proportional to the He-He cross section; Gersch and Rodriguez[15] (GR) derived a non-Lorentzian $R_{\mathrm{FS}}(Y)$ by including the effect of radial distribution function in the ground state, $g(r)$; Weinstein and Negele[16] used Brueckner theory to derive an asymptotic limit which satisfies Y scaling without the IA, and they predicted a suppression of the high-$|Y|$ components of the scattering law compared with the IA; Platzman and Tzoar[17] extended the Hohenberg-Platzman (HP) theory[9] to include the asymmetry due to the real part and the off-energy-shell behavior of the T matrix for He-He scattering at low Q, but this is negligible in the asymptotic limit; the problem has also been studied by Kirkpatrick;[18] Reiter and Becher[19] derived a Lorentzian final-state broadening for a hard-sphere system from the Chapman-Enskog equations, but with the scattering rate corrected by the value of $g(r)$ at the hard-core radius; Tanatar, Talbot, and Glyde[20] have applied the T-matrix random-phase approximation (RPA) to DINS in superfluid ^{4}He and normal ^{3}He, which also predicted an asymptotic limit having Lorentzian tails at high $|Y|$. Other theories predict no FSE broadening in the asymptotic limit: Sears[21] has proposed a series expansion for the FSE using sum rules and moments, but which suggested that the FSE vanishes at high Q as $O(Q^{-1})$; Stringari[22] has proposed that alternative Y-scaling variables could be chosen to correct for final-state effects, which included the effects of the binding of atoms in the condensed phase; Glyde[23] has used self-consistent phonon theory for solid ^{4}He to predict that the IA is accurate at Q's greater than 20 Å^{-1}. The problem has also been studied in the context of quasielastic inclusive electron-nucleus scattering.[24] Rinat[25] has provided a critical review of Sears[21] and Stringari's proposals.[22] In many of these papers,[16,20,21,23] the predicted final-state effects are not a convolution of an $R_{\mathrm{FS}}(Y)$ with an $F_{\mathrm{IA}}(Y)$. While these papers suggest many elements which may be in a complete theory, one can conclude that there is at present no theoretical consensus on final-state effects in momentum distribution experiments.

Most experiments to determine momentum distributions have been carried out at reactor neutron sources where the achievable Q's are less than 10 Å^{-1}. There have been no systematic comparisons of the various theories for FSE with experiment. However, the apparent oscillations in the width of $S(Q,\omega)$ with Q (Refs. 26 and 27) have been correlated with the well established "hard-sphere glory" oscillations in the He-He cross section[28] due to quantum statistics. A Bose-condensate fraction in ^{4}He has been inferred from experiments[29] using Q's in the range from 4 to 7 Å^{-1}. Such Q's are too low to expect the IA to be valid, and they are too low to expect most theories for FSE to hold. At these low Q's the scattering line shapes are observed to be an asymmetric function of Y, which is attributed to final-state effects. The observed scattering is symmetrized about the recoil energy to remove this asymmetric component. These symmetrized data are then analyzed for n_k. To further reduce the effect of width oscillations of the FSE with Q, the inferred n_k are averaged over several Q. These two steps correct for some consequences of the FSE expected at low Q's. Such procedures do not utilize a specific theory for FSE, nor can they be expected to completely remove FSE from the data. While the inferred values for the condensate fraction are reasonable and generally accepted, no well resolved condensate peak is observed. The data have not been compared with the IA using *ab initio* calculations of momentum distributions.[4–6]

A new generation of DINS experiments[30] is in progress at the new pulsed neutron sources which can be expected to achieve a much higher Q's (greater than 20 Å^{-1}). Such Q's are sufficiently high to compare with the asymptotic limit of the theories for FSE. The goal of the present paper is to derive a theory for $R_{\mathrm{FS}}(Y)$ in the asymptotic limit, which can be applied to the high-Q experiments on quantum solids and fluids at pulsed sources to extract momentum distributions. A successful theory for the asymptotic limit should suggest extensions to correct for FSE in low-Q experiments at reactor neutron sources.

In my view, the essential physics was included in the 1973 work by Gersch and Rodriguez,[15] who considered the effect of spatial correlations and, indeed, the two-particle density matrix (GR). A simple derivation of the effect of spatial correlations was provided by Silver and Reiter,[31] who carried out a classical trajectory calculation using Wigner's quasiclassical approximation (QC). In both papers, the physics is as follows. Before a neutron strikes a He atom, its initial position is in the attractive part of the potential well due to neighboring atoms, and it is far from the steeply repulsive core of the potential (see Fig. 1) which is responsible for final-state effects. After the neutron imparts a high momentum, the recoiling atom travels on almost a straight line until it is scattered from the repulsive core of the potential from neighboring atoms. $R_{\mathrm{FS}}(Y)$ is approximately the Fourier transform of the probability of no core collisions as a function of recoil distance. Since there are no collisions at short recoil distances due to the initial spatial correlations, there should be no high-$|Y|$ (Lorentzian) tails on $R_{\mathrm{FS}}(Y)$, and the broadening should be narrower than the Lorentzian broadening theories which correspond to setting $g(r) \rightarrow 1$.

As I shall show in Sec. V, the QC (Ref. 31) and the GR (Ref. 15) theories produce a mathematical form for $R_{\mathrm{FS}}(Y)$ involving $g(r)$ which is similar to what I obtain in the "hard-core perturbation theory" (HCPT) to be developed below. However, the three theories differ in the effective classical trajectory to be used in calculating $R_{\mathrm{FS}}(Y)$, as well as in other important ways. For exam-

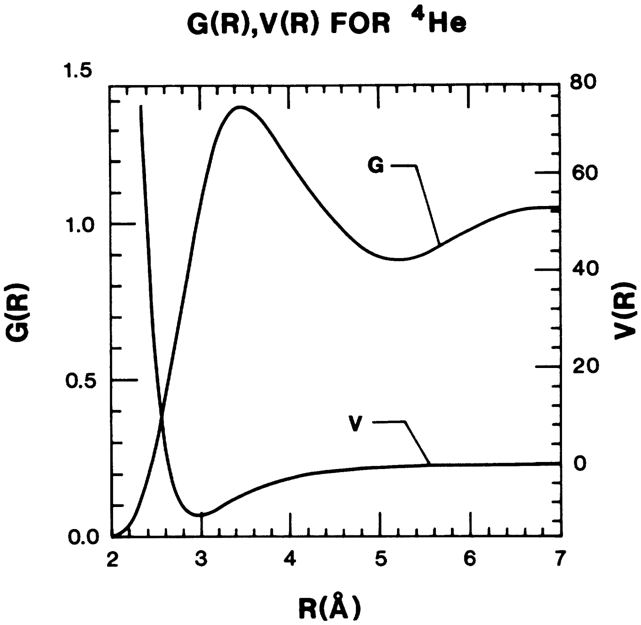

FIG. 1. Plot of the radial distribution function, $g(r)$, for superfluid ^{4}He and the He-He potential, $V(r)$.

ple, in the QC calculation the cross section for a hard sphere is πr_0^2 instead of $2\pi r_0^2$, and the recoil momentum is $Q/2$ instead of Q.

This paper is the first of two to present details of the first perturbative calculation[1] of the final-state corrections in DINS experiments which includes the effect of the spatial correlations. The present paper presents the many-body formalism for the derivation of $R_{\rm FS}(Y)$ using a combination of Liouville perturbation theory and off-diagonal projection superoperators, which I term hard-core perturbation theory (HCPT). While these methods are somewhat novel, they have a strong theoretical precedent[32–34] in the perturbative derivation of the Boltzmann-equation expression for the electrical resistivity in a metal due to impurity scattering starting from the Kubo (linear-response) formula for the electrical conductivity. An analogous procedure will be developed for $S(Q,\omega)$ in this paper. The methods are also related to the Singwi, Tosi, Land, and Sjolander[35] (STLS) scheme for electron correlations, an analogy which will be developed elsewhere.[36] The "purist" might argue that, in principle, the present results should be obtained via Green's-function methods which invoke Ward identities to relate vertex functions to two-particle density matrices.[37] However, I doubt that such a derivation would add to the physics.

I derive very simple expressions for $R_{\rm FS}(Y)$ which involve the He-He phase shifts and $g(r)$. These expressions meet all the requirements for a quantum theory first discussed by Silver and Reiter.[31] They satisfy the f, ω^2, and ω^3 sum rules. Moreover, the results have a compelling physical rationale independent of the details of the derivations. In order to put these new results into context, I will compare the HCPT theory to most of the prior theories of DINS experiments including the IA, Lorentzian broadening (LZ), t-matrix RPA (RPA), quasiclassical models (QC), Gersch and Rodriguez's[15] many-body cumulant expansion (GR), etc. The expression of final-state effects in DINS in terms of $g(r)$ and phase shifts is reminiscent of extended x-ray-absorption fine structure (EXAFS) (Ref. 38) theory.

Section II introduces the general formalism of superoperators and Liouville perturbation theory, which has previously seen important applications in transport theory. Section III specializes to the derivation of a HCPT Dyson equation valid in the limit of high Q and ω. Section IV presents a discussion of sum rules, properties of the t matrix, and the relation to the IA, LZ, and RPA theories for DINS. In Sec. V, the Dyson equation is solved by semiclassical methods to arrive at the final expressions for $R_{\rm FS}(Y)$. The $O(Q^{-1})$ corrections to the theory are discussed along with the relation to the QC and GR theories. Section VI concludes and discusses the theory for DINS experiments in quantum solids and fluids.

In a subsequent paper,[2] massive numerical predictions are presented for DINS experiments in superfluid ^{4}He.

II. LIOUVILLE PERTURBATION THEORY AND SUPEROPERATOR FORMALISM

The problem of deriving the Boltzmann-equation expression for the resistivity starting from the Kubo expressions for the frequency-dependent conductivity in a metal, $\sigma(\omega)$, is in many ways formally analogous to the problem of evaluating the neutron scattering law, $S(Q,\omega)$. One starts with

$$\sigma(\omega)\equiv \int_0^\infty dt\, e^{i\omega t-\varepsilon t}\langle e^{i\hat{H}t}\mathbf{v}(0)e^{-i\hat{H}t}\cdot\mathbf{v}(0)\rangle \ . \tag{1}$$

Here $\mathbf{v}(0)$ is the velocity operator. A naive expansion of the time-dependent part of (1) will result in an infinite number of terms which diverge as inverse powers of $\omega+i\varepsilon$. A method for infinite-order resummation is essential. A solution to this problem is to use Liouville perturbation theory and diagonal projection superoperators.[32–34]

An operator, $\hat{O}$, is composed of sums of products of creation and annihilation operators with scalars. A "superoperator," $\tilde{S}$, acts on an ordinary operator to its right to create a new operator, according to $\tilde{S}\hat{O}\equiv\hat{O}'$. The Liouville superoperator, $\tilde{L}$, is defined by $\tilde{L}\hat{O}\equiv-[\hat{H},\hat{O}]$. $\tilde{L}$ can be written as the sum of kinetic, $\tilde{K}$, plus potential $\tilde{V}$, terms. Then the time evolution of any operator can be written

$$\hat{O}(\omega)\equiv\int_0^\infty dt\, e^{i\omega t-\varepsilon t}e^{i\hat{H}t}\hat{O}(0)e^{-i\hat{H}t} = \frac{i}{\omega-\tilde{L}+i\varepsilon}\hat{O}(0) \tag{2}$$

which can be expanded as a Dyson equation

$$\hat{O}(\omega)=\frac{i}{\omega-\tilde{K}+i\varepsilon}[\hat{O}(0)+\tilde{V}\hat{O}(\omega)] \ . \tag{3}$$

For example, consider the Kubo formula, Eq. (1), with the velocity operator defined by

$$\mathbf{v}(0) \equiv \sum_k \frac{\mathbf{k}}{m} \hat{a}_k^\dagger \hat{a}_k \ . \tag{4}$$

The perturbative expansion of $\hat{\mathbf{v}}(\omega)$ as in Eq. (3) results in an infinite number of terms which are singular as inverse powers of $\omega+i\varepsilon$ as $\omega-\tilde{K}+i\varepsilon$ acts on components of $\tilde{V}\hat{\mathbf{v}}(\omega)$ of the form $\hat{a}_k^\dagger \hat{a}_k$.

The neutron scattering law, $S(Q,\omega)$, is formally analogous to the Kubo formula. That is

$$S(Q,\omega) \equiv \frac{\mathrm{Re}}{\pi N} \langle \hat{\rho}^{Q}(\omega) \hat{\rho}^{-Q}(0) \rangle, \quad \hat{\rho}^{Q}(0) \equiv \sum_k \hat{a}_k^\dagger \hat{a}_{k+Q} \ . \tag{5}$$

The perturbative expansion of $\hat{\rho}^{Q}(\omega)$ as in Eq. (3) results in an infinite number of terms which are singular as inverse powers of $\omega - Q^2/2m + i\varepsilon$ as $\omega - \tilde{K} + i\varepsilon$ acts on components of $\tilde{V}\hat{\rho}^{Q}(\omega)$ of the form $\hat{a}_k^\dagger \hat{a}_{k+Q}$. The behavior of $S(Q,\omega)$ as $\omega \to Q^2/2m$ is precisely what is important to DINS experiments. It is apparent that methods which have been applied to the perturbative evaluation of the Kubo formula should also be applicable to DINS.

The singular terms in the Kubo formula are resummed by what is known as the "diagonal projection superoperator" method.[32–34] One argues that only the most singular terms as $\omega \to 0$ in the perturbative expansion of the Kubo formula need be retained, i.e., those parts of $\hat{\mathbf{v}}(\omega)$ which have the form $\hat{a}_k^\dagger \hat{a}_k$. A superoperator, $\tilde{\Delta}$, is defined which when acting on any operator, $\hat{O}$, retains only those components of the form $\hat{a}_k^\dagger \hat{a}_k$ which produce the singular terms, i.e.,

$$\tilde{\Delta}\hat{O} \equiv \sum_k O_k \hat{a}_k^\dagger \hat{a}_k \ , \tag{6}$$

where the coefficients O_k are scalars. It is "diagonal" because the arguments of the creation and annihilation operators in its definition, Eq. (6), are the same. Analogously, for the neutron scattering case one would seek an "off-diagonal" superoperator for the terms of the form $\hat{a}_k^\dagger \hat{a}_{k+Q}$ which are singular as $\omega \to Q^2/2m$, i.e.,

$$\tilde{\Delta}\hat{O} \equiv \sum_k O_k \hat{a}_k^\dagger \hat{a}_{k+Q} \ . \tag{7}$$

$\tilde{\Delta}$ is a "projection" superoperator, which means it must satisfy $\tilde{\Delta}\tilde{\Delta} = \tilde{\Delta}$ and $\tilde{\Delta}\hat{O}(0) = \hat{O}(0)$. One defines its complement by $\tilde{\Delta}' \equiv 1 - \tilde{\Delta}$. Using the general properties of projection superoperators, and not the specific form of Eqs. (6) or (7), it is a matter of straightforward manipulations[33] to derive from Eq. (3)

$$\tilde{\Delta}\hat{O}(\omega) = \frac{1}{\omega - \tilde{K} + i\varepsilon} [i\hat{O}(0) + \tilde{\Delta}\tilde{T}\tilde{\Delta}\tilde{\Delta}\hat{O}(\omega)] \ , \tag{8}$$

where

$$\tilde{T} \equiv \tilde{V} + \tilde{V}\tilde{\Delta}' \frac{1}{\omega - \tilde{K} - \tilde{\Delta}'\tilde{V}\tilde{\Delta}' + i\varepsilon} \tilde{\Delta}'\tilde{V}\tilde{\Delta} \ . \tag{9}$$

This reordering of the perturbation expansion is exact for any projection superoperator, $\tilde{\Delta}$, and for any operator, $\hat{O}$. Remember that all superoperators act sequentially on operators to their right. The first $\tilde{\Delta}$ indicates that $\tilde{\Delta}\tilde{T}\tilde{\Delta}$ acts on an initial operator of the form $\hat{a}_{k'}^\dagger \hat{a}_{k+Q}$ while the final $\tilde{\Delta}$ requires that the final result contains only operators of the form $\hat{a}_{k'}^\dagger \hat{a}_{k'+Q}$. Therefore, $\tilde{\Delta}\tilde{T}\tilde{\Delta}$ can be represented in terms of scalar components of a dyadic, $\bar{T}_{k,k'}$. Then Eq. (8) yields an integral equation for the coefficients O_k

$$O_k(\omega) = \frac{1}{\omega - \delta e_k + i\varepsilon} \left[iO_k(0) + \sum_{k'} \bar{T}_{k,k'} O_{k'}(\omega) \right] . \tag{10}$$

δe_k is 0 for the Kubo formula and is $e_{k+Q} - e_k$ for $S(Q,\omega)$.

The first approximation then for both the Kubo formula and $S(Q,\omega)$ has the form

$$\langle \hat{O}(\omega) \hat{O}^\dagger(0) \rangle \to \langle \tilde{\Delta}\hat{O}(\omega) \hat{O}^\dagger(0) \rangle \tag{11}$$

which retains all the most singular terms. The second approximation is to the $\bar{T}_{k,k'}$, which depends on the specific physics of the problem. This amounts to a choice for the truncation of the continued fraction expansion indicated by Eqs. (2), (8), and (9) and a choice for the projection superoperator $\tilde{\Delta}$.

Consider the problem of evaluating the Kubo formula for weak impurity scattering in a metal. Then the potential is

$$\hat{V} \equiv \sum_j \sum_{k,q} V(q) \hat{a}_{k+q}^\dagger \hat{a}_k e^{iqr_j} \ . \tag{12}$$

Here the summation over j means a summation over all the impurities in the system. The usual treatment is to take the expectation value, $\langle \ \ \rangle$, to mean an average with respect to the "noninteracting" ground state, to take $\tilde{\Delta}$ to be the same as an average over impurity positions, and to retain terms to only second order in V in Eq. (9). Then the first term in (9) is zero provided $V(q=0)=0$, and the second term in (9) gives

$$\bar{T}_{k\neq k'} = -N_I V^2(k-k') \times \left[\frac{1}{\omega - e_k + e_{k'} + i\varepsilon} + \frac{1}{\omega + e_k - e_{k'} + i\varepsilon} \right] \tag{13}$$

and

$$\bar{T}_{k,k} = -\sum_{k'(\neq k)} \bar{T}_{k,k'} \ , \tag{14}$$

where N_I is the number of impurities. Sometimes, $V(q)$ in Eq. (13) is replaced by the single-particle t matrix in the case of strong but dilute scatterers. Terms of the form of Eq. (13) may be labeled vertex terms, whereas terms of the form of Eq. (14) may be labeled "self-energy" terms. When (13) and (14) are substituted into Eq. (10) and the limit $\omega \to 0$ taken, the result is the usual Boltzmann equation whose solution for the resistivity is in standard textbooks.[39] There are important cancellations between vertex and self-energy terms which lead to the familiar $1 - \cos\theta_{k,k'}$ factor in the Boltzmann formula for the resistivity. Such cancellations will also be important to the theory of DINS, for, as we shall see, the improper neglect of vertex terms will lead to the Lorentzian broadening theories.

Clearly, helium is a strongly interacting system. A perturbation theory for $S(Q,\omega)$ starting from noninteracting ground states, such as the above treatment of the Kubo formula in the limit of weak impurity scattering, is sure to be slowly convergent. A perturbation theory for the dynamical response in helium starting from the static properties of the strongly interacting system, such as $g(r)$ and n_k taken from experiment or other many-body theory, is more likely to be rapidly convergent. To develop this, a projection superoperator should be chosen which can be extended to expectation values, $\langle\ \rangle$, in "interacting" ground states, $|\Psi_0\rangle$, rather than noninteracting ones.

I define such an off-diagonal projection superoperator, $\tilde{\Delta}$, appropriate to the important singularities in $S(Q,\omega)$, as follows

$$\tilde{\Delta}\hat{O}\equiv\sum_k \hat{a}_k^\dagger\hat{a}_{k+Q}\frac{\langle[(\hat{a}_k^\dagger\hat{a}_{k+Q})^\dagger,\hat{O}]\rangle}{n_{k+Q}-n_k} . \tag{15}$$

Here $\langle\ \rangle$ denotes expectation value in the fully interacting ground state, and $[\hat{A},\hat{B}]$ is a commutator. It is readily verified that Eq. (15) satisfies the projection superoperator requirements $\tilde{\Delta}\tilde{\Delta}=\tilde{\Delta}$ and $\tilde{\Delta}\hat{a}_k^\dagger\hat{a}_{k+Q}=\hat{a}_k^\dagger\hat{a}_{k+Q}$. Remarkably, the same projection superoperator is valid for both fermions and bosons. It also works when $\langle\ \rangle$ denotes an ensemble average. $\tilde{\Delta}$ acting on any operator projects out only those components of the operator which produce single particle-hole excitations out of the ground state.

This projection superoperator can be applied to the Kubo formula for weak impurity scattering to yield identical results to Eqs. (13) and (14) when $\tilde{\Delta}$ is augmented by an impurity average and the $Q\rightarrow 0$ is taken at the end of the manipulations.

III. DERIVATION OF A DYSON EQUATION FOR DEEP INELASTIC NEUTRON SCATTERING

The previous section has identified the formal analogy between the perturbative evaluation of Kubo expressions for transport coefficients and the evaluation of the neutron scattering law at high Q and ω. In both cases, a naive expansion results in an infinite number of divergent terms which must be resummed to all orders by some method. I have suggested that Liouville perturbation theory with an appropriate choice of projection superoperator may provide an appropriate method. However, in helium the starting point of the perturbation expansion should be the strongly interacting ground state. A possible projection superoperator for helium, Eq. (15), has been proposed. In this section, I combine these formal developments with the physics to derive a Dyson equation for DINS. In the following, I explicitly consider ^{4}He so that all creation and annhilation operators are bosons.

There are different momentum and distance scales in the DINS problem. The characteristic momenta of the helium many-body system can be characterized by q's such that $n_q\neq 0$ and $\int d^3r e^{iqr}[g(r)-1]\neq 0$. The momentum imparted by a neutron to the recoiling He atom in a DINS experiment is much larger than these characteristic values. This allows a clear separation of the problem into high (Q) and low (q) momenta. There are also different time and energy scales in the problem. The final-state interactions are due to the collisions of recoiling high-Q helium atoms with the steeply repulsive cores of the potentials on initially low-q neighboring atoms. These collisions occur on a time scale which is very short and an energy scale which is very high compared with the longer-range and lower-energy interactions responsible for the collective excitations and the structure of helium. These collisions can therefore be regarded as two-body, and many-body and collective effects can be ignored.

The goal of the present theory is to capture the leading behavior at high Q of the final-state effects in helium, which is applicable to the analysis of DINS data from pulsed neutron sources. ^{4}He is an almost hard-sphere system, with the He-He cross section "glory" oscillating about an average which decreases logarithmically with increasing Q. For a true hard-sphere system, the cross section is constant at very high Q, and Y scaling will be obtained without the IA. In the spirit of deriving the asymptotic limit of the FSE discussed in the Introduction, I drop terms of $O(Q^{-1})$ which are not present in the limit of hard-core short-range potentials and $Q\rightarrow\infty$. The effects of such lower-energy (longer-range) components of the interaction are only to determine the initial conditions (ground-state wave function) before the scattering of a neutron, i.e., the n_k and $g(r)$. The extension to experiments on helium at large but finite Q is straightforward, and is presented in Sec. IV.

These physical ideas motivate the approximations of the present theory, which are:

(a) to keep only the most singular terms as $\omega\rightarrow Q^2/2m$;

(b) to include only the dynamics of the high-Q particles;

(c) to consider only two-body collisions;

(d) to treat "low"-k particles statically in terms of their initial spatial correlations as expressed by $g(r)$ and initial momentum distributions as expressed by n_k;

(e) keep only terms which Y scale in the asymptotic limit (hard-core short-range potential as $Q\rightarrow\infty$), i.e., drop terms of $O(Q^{-1})$.

These physical ideas imply that the collective behavior and long-range order in the condensed state are irrelevant to final-state broadening of the IA. Thus, the present theory should be valid for solids as well as fluids, fermions as well as bosons, etc. with the $g(r)$ and n_k as the only important ground-state variables.

To translate these ideas into mathematics, consider the calculation of $S(Q,\omega)$, Eq. (5), within *only the most singular terms approximation*, (a), as given by Eq. (11). I can write

$$\tilde{\Delta}\hat{\rho}^Q(\omega)\equiv\sum_k S_k^Q(\omega)\hat{a}_k^\dagger\hat{a}_{k+Q} , \tag{16}$$

where the $S_k^Q(\omega)$ are scalar coefficients. Then using Eqs. (5) and (11),

$$S(Q,\omega)=\frac{\mathrm{Re}}{\pi N}\sum_k\sum_{k'}S_k^Q(\omega)\langle\hat{a}_k^\dagger\hat{a}_{k+Q}\hat{a}_{k'+Q}^\dagger\hat{a}_{k'}\rangle . \tag{17}$$

The $\langle\ \rangle$ represents expectation values in a strongly interacting ground-state $|\Psi_0\rangle$. This has no high-momentum components so that $\hat{a}_Q\,|\,\Psi_0\rangle=0$ for any high momentum, Q. Therefore, $S(Q,\omega)$ simplifies to

$$\lim_{\text{high } Q} S(Q,\omega)\rightarrow \frac{\text{Re}}{\pi N}\sum_k S_k^Q(\omega)n_k \ . \tag{18}$$

Because of the n_k in Eq. (18), only $S_k^Q(\omega)$ for low momenta k should be considered. These come from a solution of an integral equation for $\tilde{\Delta}\hat{\rho}^Q(\omega)$ analogous to Eq. (8) using the appropriate projection superoperator, Eq. (15). The physics is in the approximations for $\tilde{\Delta}\tilde{T}\tilde{\Delta}$ in terms of scalar coefficients $\overline{T}_{k,k'}$ as in Eq. (10) referred to operators of the form $\hat{a}_{k'}^{\dagger}\hat{a}_{k+Q}$ and $\hat{a}_{k'}^{\dagger}\hat{a}_{k'+Q}$.

The *high-momentum dynamics only* approximation, (b), is implemented by allowing $\tilde{T}$ to act only on the $\hat{a}_{k+Q}$, i.e.,

$$\tilde{T}\hat{a}_k^{\dagger}\hat{a}_{k+Q}\rightarrow \hat{a}_k^{\dagger}(\tilde{T}\hat{a}_{k+Q}) \ . \tag{19}$$

The *two-body collision approximation,* (c), is implemented by replacing the many-body $\tilde{T}$ superoperator, Eq. (9), by a two-body $\tilde{T}$ superoperator given by

$$\tilde{T}\hat{O}\rightarrow -[\hat{T}_2,\hat{O}] \tag{20}$$

such that

$$\hat{T}_2\equiv\frac{1}{2\Omega}\sum_{k_1,k_2,q}\hat{a}_{k_1+q}^{\dagger}\hat{a}_{k_2-q}^{\dagger}T_{k_1k_2q}\hat{a}_{k_2}\hat{a}_{k_1} \tag{21}$$

where Ω is volume, and the $T_{k_1k_2q}$ are scalar coefficients given by the two-body t matrix. The operator component of $\hat{T}_2$ is exactly like the two-body potential

$$\hat{V}\equiv\frac{1}{2\Omega}\sum_{k_1,k_2,q}\hat{a}_{k_1+q}^{\dagger}\hat{a}_{k_2-q}^{\dagger}V(Q)\hat{a}_{k_2}\hat{a}_{k_1} \ . \tag{22}$$

However, $\hat{T}_2$ includes the interaction between the two particles to all orders in the potential. On-energy shell, the $T_{k_1k_2q}$ can be expressed in terms of the He-He phase shifts, to be discussed in more detail in Sec. IV.

Approximation (d), *treat low-momentum particles statically in terms of their ground-state spatial correlations and momentum distributions,* is implemented by the choice of projection superoperator, $\tilde{\Delta}$. It projects out expectation values of operators in the ground-state wave function, $|\,\Psi_0\rangle$. More specifically, the two-body collision approximation, Eq. (21), and choice of projection superoperator, Eq. (15), yields via Eq. (10) a closed system of equations for the $S_k^Q(\omega)$,

$$S_k^Q(\omega)=\frac{1}{\omega-e_{k+Q}+i\varepsilon}\left[i+\sum_{k'}\overline{T}_{k,k'}S_{k'}^Q(\omega)\right] \ . \tag{23}$$

Here the e_k has been ignored because it is $O(Q^{-1})$.

The final element needed to complete the derivation of a Dyson equation for DINS is the explicit calculation of the $\overline{T}_{k,k'}$ in Eq. (23) using Eqs. (15) and (19)–(21). After several pages of straightforward (albeit tedious) algebra with no further approximations, one arrives at four terms. Without going into excessive detail, it is easy to see what happens. The first $\tilde{\Delta}$ forces the initial operator to have the form $\hat{a}_k^{\dagger}\hat{a}_{k+Q}$. The $\tilde{T}$ commutes a product of two $\hat{a}^{\dagger}$ and two $\hat{a}$ with this resulting in a new operator with two $\hat{a}^{\dagger}$ and two $\hat{a}$. The second $\tilde{\Delta}$ first commutes an operator of form $(\hat{a}_k^{\dagger}\hat{a}_{k+Q})$, still leaving two $\hat{a}^{\dagger}$ and two $\hat{a}$. Finally, the expectation value is taken in the ground state. The result is that the $\overline{T}_{k,k'}$ involve sums over products of the $T_{k_1k_2q}$ with the ground-state expectation values of the two-particle density matrix

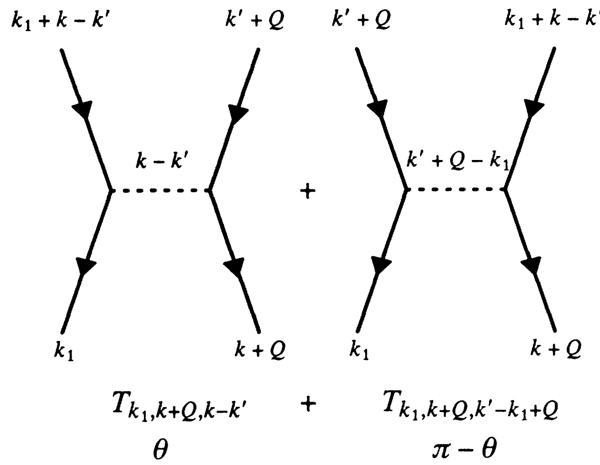

FIG. 2. Diagrammatic representation of the t matrices, $T^B_{k_1k_2q}$, which occur in the Dyson equation for DINS, Eq. (29).

$$\Phi_{k_1k_2q}\equiv\langle\hat{a}_{k_1+q}^{\dagger}\hat{a}_{k_2-q}^{\dagger}\hat{a}_{k_2}\hat{a}_{k_1}\rangle \ . \tag{24}$$

The $\Phi_{k_1k_2q}$ are related to the radial distribution function, $g(r)$, and the momentum distribution, n_k, by sum rules, i.e.,

$$\frac{1}{N}\sum_{k_1,k_2}\Phi_{k_1k_2q}=\rho\int d^3r\, e^{iqr}g(r) \ , \tag{25}$$

where ρ is the particle density, and

$$\lim_{q\to 0}\frac{1}{N}\sum_{k_2}\Phi_{k_1k_2q}=n_{k_1} \ . \tag{26}$$

If any of the arguments of $\Phi_{k_1k_2q}$ is a "high" momentum, then $\Phi_{k_1k_2q}$ is zero by definition. Finally, we note a symmetry relation for bosons

$$\Phi_{k_1k_2Q}=\Phi_{k_1k_2K},\quad K=k_2-Q-k_1 \ . \tag{27}$$

Two of the four terms can be eliminated because the arguments of $\Phi_{k_1k_2q}$ involve high momenta. The n_{k+Q} in the definition of the projection superoperator, Eq. (15), is also zero at high Q. The final result is

$$\overline{T}_{k,k'}=\frac{1}{\Omega n_k}\sum_{k_1}(T_{k_1,k+Q,k-k'}+T_{k_1,k+Q,k'-k_1+Q})\Phi_{k_1,k,k-k'} \ . \tag{28}$$

The two terms in this equation add with a plus sign because of Bose symmetry. They correspond to the addition of t matrices for scattering angles θ and $\pi-\theta$, which eliminates all odd partial waves in the phase shift analysis of $T_{k_1k_2q}$. A diagrammatic representation of these t matrices is shown in Fig. 2. I label this Bose-symmetrized t matrix $T^B_{k_1k_2q}$. Then the final HCPT Dyson equation for the $S^Q_k(\omega)$ in the limit of high Q is

$$S^Q_k(\omega)=\frac{1}{\omega-e_{k+Q}+i\varepsilon}\left[i+\frac{1}{\Omega n_k}\sum_{k',k_1}T^B_{k_1,k+Q,k-k'}\Phi_{k_1,k,k-k'}S^Q_{k'}(\omega)\right] . \tag{29}$$

The small parameter of this perturbation expansion is the product of $T_{k_1k_2q}$ and $\Phi_{k_1k_2q}$, which is well behaved at high momenta and short distances. Philosophically, the hard-core components of the potential have been screened by the ground-state correlations. This justifies the oxymoron, hard core perturbation theory. I shall show in Sec. IV that many of the previous theories for DINS can be obtained as approximations to Eq. (29). Section V presents a semiclassical solution to Eq. (29) within an approximation for the two-particle density matrix, Φ.

For ^{3}He, the result would be Eq. (29) with an antisymmetrized $T^F_{k_1k_2q}$ and $\Phi_{k_1k_2q}$ for Fermi statistics, and with spin arguments added to $T^F_{k_1k_2q}$ and $\Phi_{k_1k_2q}$. ^{3}He will be discussed in more detail in a separate paper.[40]

IV. SUM RULES, THE T MATRIX, AND RELATION TO OTHER THEORY

The physics in Eq. (29) can be brought out by considering the IA limit, the sum rules on $S(Q,\omega)$, the properties of the t matrix, and relation to the alternative theories for DINS. First, if I take the limit of no final state scattering, $T^B_{k_1k_2q}\rightarrow 0$, then the impulse approximation (IA) for $S(Q,\omega)$ is recovered

$$S_{\rm IA}(Q,\omega)=\frac{1}{\rho}\int\frac{d^3k}{(2\pi)^3}n_k\delta\left[\omega-\frac{Q^2}{2M}-\frac{kQ}{M}\right] . \tag{30}$$

The Y scaling form of the IA can be written in terms of the components of k parallel, $k_\parallel$, and perpendicular, $k_\perp$, to Q and $Y\equiv M(\omega-Q^2/2M)/Q$.

$$F_{\rm IA}(Y)\equiv\frac{QS_{\rm IA}(Q,\omega)}{M}=\frac{1}{\rho}\int\frac{d^2k_\perp dk_\parallel}{(2\pi)^3}n(k_\parallel,k_\perp)\delta(Y-k_\parallel) . \tag{31}$$

Here $n(k_\parallel,k_\perp)\equiv n_k$. Thus in the IA the scaling variable, Y, corresponds to the parallel component of the momentum distribution. $F_{\rm IA}(Y)$ is normalized to unit integral over Y.

In the limit of high Q, it is straightforward to show that the sum rules[23] on $S(Q,\omega)$ simplify to

$$f \text{ sum rule}\rightarrow\int_{-\infty}^{\infty}YF(Y)dY=0 , \tag{32a}$$

$$\omega^2 \text{ sum rule}\rightarrow\int_{-\infty}^{\infty}Y^2F(Y)dY=\frac{2M}{3}\langle E_{\rm KE}\rangle , \tag{32b}$$

$$\omega^3 \text{ sum rule}\rightarrow\int_{-\infty}^{\infty}Y^3F(Y)dY=O(Q^{-1}) . \tag{32c}$$

Here, $O(Q^{-1})$ in Eq. (32c) means that it goes to zero with increasing Q at least as fast as Q^{-1}. In the spirit of approximation (e), the test will be whether the asymptotic limits (hard-core short-range potential as $Q\rightarrow\infty$) of the various theories satisfy these sum rules. If the final-state broadening can be represented by a convolution of an $R_{\rm FS}(Y)$ with $F_{\rm IA}(Y)$, then the sum rules are equivalent to

$$f \text{ sum rule}\rightarrow\int_{-\infty}^{\infty}YR_{\rm FS}(Y)dY=0 , \tag{33a}$$

$$\omega^2 \text{ sum rule}\rightarrow\int_{-\infty}^{\infty}Y^2R_{\rm FS}(Y)dY=0 , \tag{33b}$$

$$\omega^3 \text{ sum rule}\rightarrow\int_{-\infty}^{\infty}Y^3R_{\rm FS}(Y)dY=O(Q^{-1}) , \tag{33c}$$

Eq. (33b) clearly rules out Lorentzian wings on $R_{\rm FS}(Y)$.

We shall also need the properties of the t matrix, $T^B_{k_1k_2q}$. In terms of variables of the center of mass (c.m.) frame for the collision, when the t matrix is on-energy shell it can be represented in terms of partial waves

$$T^B_{k_1k_2q}\equiv t(k_{\rm c.m.},\theta)=-\frac{4\pi}{2\mu ik_{\rm c.m.}}\sum_{l\ \rm even}(2l+1)(e^{2i\delta_l}-1)P_l(\cos\theta) , \tag{34}$$

where $\mu\equiv M/2$ is reduced mass, the particle momentum $k_{\rm c.m.}\equiv(k_1-k_2)/2$ determines the phase shifts δ_l, and θ is the scattering angle. The forward t matrix, $\theta=0$, is related to the total cross section

$$\sigma_{\rm tot}\equiv\frac{4\pi}{k^2_{\rm c.m.}}\sum_{l=0}^{\infty}(l+\tfrac{1}{2})[1-\cos(2\delta_l)] \tag{35}$$

by the optical theorem

$$\mathrm{Im}T_{k_1k_20} = -\frac{k_{\mathrm{c.m.}}}{2\mu}\sigma_{\mathrm{tot}} . \tag{36}$$

In the asymptotic limit, the summation over partial waves in Eqs. (34) and (35) can be converted to an integral over impact parameters

$$b \equiv \left[l + \frac{1}{2} \right] \frac{2}{Q} . \tag{37}$$

At high Q, the phase shifts may be accurately evaluated using the Langer form of the Jeffreys-Wentzel-Kramers-Brillouin (JWKB) approximation

$$\delta_l \simeq \int_{r_0}^{\infty} dr \left[\left[2\mu[E - V(r)] - \frac{L^2}{r^2} \right]^{1/2} - \sqrt{2\mu E} \right] - \sqrt{2\mu E}\, r_0 + \frac{L\pi}{2} . \tag{38}$$

Here r_0 is the classical turning point of the trajectory and $L = l + \frac{1}{2}$. Equivalently,

$$\delta_b = \frac{Q}{2} \left\{ \int_{r_0}^{\infty} dr \left[\left[1 - V'(r) - \frac{b^2}{r^2} \right]^{1/2} - 1 \right] - r_0 + \frac{b\pi}{2} \right\} , \tag{39}$$

where $V' = 4MV/Q^2$. Here, the classical turning point is defined by $1 - V'(r_0) - b^2/r_0^2 = 0$. For a potential which is strictly hard core at short range, in the asymptotic limit r_0 is independent of b. The exponential of $2i\delta_b$ phase oscillates to zero for $b < r_0$ and is one for $b > r_0$.

To extend the asymptotic limit result to predict FSE for the steeply repulsive He-He potential at finite Q, one can calculate a Q-dependent r_0. This will decrease as $\ln Q$ at high Q for a potential which has the form $V'(r) \propto e^{-ar}$ at short distances. More generally, one can simply retain the full phase shift analysis which will retain certain terms of $O(Q^{-1})$. In addition to the $\ln Q$ decrease of the average of σ_{tot}, the $O(Q^{-1})$ terms produce "glory" oscillations about the average whose phase depends on quantum statistics.[41] This will be discussed further in Sec. V.

The specific quantity of interest in Eq. (29) is $T^B_{k_1,k+Q,q}$. At high Q, the phase shifts are independent of k and k_1 and depend only on $k_{\mathrm{c.m.}} \to Q/2$. The scattering angle becomes

$$\theta \simeq 2\frac{q_\perp}{Q} . \tag{40}$$

Then, one can write

$$\lim_{\text{high } Q} T^B_{k_1,k+Q,q} = t(k_{\mathrm{c.m.}},\theta) \to t(Q/2, 2q_\perp/Q) . \tag{41}$$

The real part of $T^B_{k_1,k+Q,q}$ is small.

The integral equations of the form of Eq. (10) and (29) are examples of an exact relation for the components of the susceptibility

$$\chi(Q,\omega) = i\langle[\hat\rho^{Q}(\omega), \hat\rho_{-Q}(0)]\rangle ,$$
$$\chi_k(Q,\omega) = i\langle[\hat\rho^{Q}(\omega), \hat a^\dagger_{k+Q}\hat a_k]\rangle . \tag{42}$$

In particular, the χ_k satisfy an exact relation of the form

$$\chi_k = \chi_k^0 + \chi_k^0 \frac{1}{\Omega} \sum_{k'} I(k,k')\chi_{k'} \tag{43}$$

and they are related to the $S_k^0(\omega)$ by

$$S_k^Q(\omega) = i\frac{\chi_k(Q,\omega)}{n_{k+Q} - n_k} . \tag{44}$$

In HCPT, the kernel is

$$I_{\mathrm{HCPT}}(k,k') = -\frac{1}{n_k n_{k'}} \sum_{k_1} T^B_{k_1,k+Q,k-k'} \Phi_{k_1,k,k-k'} . \tag{45}$$

The alternative theories differ in the choice of kernel, $I(k,k')$, and in their predictions for FSE in the asymptotic limit.

The theories of Hohenberg and Platzman[9] and Platzman and Tzoar[17] (labeled LZ for Lorentzian) can be obtained by taking the limit of a structureless fluid, $g(r) \to 1$, which corresponds to $\Phi_{k_1k_2q} \to n_{k_1}n_{k_2}\delta_{q=0}$. That is

$$I_{\mathrm{LZ}}(k,k') = -\frac{\delta_{k-k'}}{n_{k'}} \sum_{k_1} n_{k_1} T^T_{k_1,k+Q,0} . \tag{46}$$

Then Eq. (29) has the solution

$$\lim_{g(r)\to 1} S_k^Q(\omega) = \frac{i}{\omega - e_{k+Q} - \frac{1}{\Omega}\sum_{k_1} n_{k_1} T^B_{k_1,k+Q,0}} . \tag{47}$$

This has the form of a self-energy correction to the propagator for a high Q particle. Applying the properties of the t matrix discussed in the previous paragraph, one has in the asymptotic limit

$$S_k^Q(\omega) \approx \frac{i}{\omega - \frac{Q^2}{2M} - \frac{k_\parallel Q}{M} + \frac{i\rho Q}{2M}\sigma_{\mathrm{tot}}(Q)} . \tag{48}$$

Substituting this into Eq. (18), using the Y-scaling variable, and Eq. (31), it is straightforward to derive the LZ prediction of a convolution

$$F_{\rm LZ}(Y)\equiv\frac{Q}{M}S(Q,\omega)=\int_{-\infty}^{\infty}dY'R_{\rm LZ}(Y-Y')F_{\rm IA}(Y')\ , \tag{49}$$

where the final state broadening function, $R_{\rm LZ}(Y)$, has Lorentzian form

$$R_{\rm LZ}(Y)=\frac{1}{\pi}\frac{\Gamma}{Y^2+\Gamma^2},\quad \Gamma=\frac{\rho}{2}\sigma_{\rm tot}\ . \tag{50}$$

While LZ satisfies the f sum rule and ω^3 sum rules, it does not satisfy the ω^2 ("kinetic energy") sum rule in the asymptotic limit. Extending this theory to a steeply repulsive He-He potential at finite Q leads to the width oscillations which have been experimentally observed at low Q.[41] An emphasis in Platzman and Tzoar's paper[17] was on the importance of the off-energy-shell behavior and real part of $T^B_{k_1k_2q}$ leading to an asymmetry in the line shape. However, this effect is negligible in the asymptotic limit.

Another theory for final state broadening invokes the t-matrix random-phase approximation.[20]

$$I_{\rm RPA}(k,k')\rightarrow -T^B_{k,k'+Q,Q}\ . \tag{51}$$

The emphasis in this paper was on interpreting the width oscillations which are observed at $Q<10$ Å^{-1}. For ^{3}He $T^F_{k_1k_2q}$ is the solution of a Galitskii-Feynman theory taking into account the occupation factors, n_k. In the asymptotic limit, the occupation factors are unimportant and the Galitskii-Feynman and free-particle forms of $T^F_{k_1k_2q}$ or $T^B_{k_1k_2q}$ converge. Ignoring the small real part of the $T^B_{k_1k_2q}$, one obtains the usual RPA

$$\chi(Q,\omega)\simeq\frac{\chi^0(Q,\omega)}{1-i\dfrac{Q\pi\rho}{2M}\sigma_{\rm tot}\chi^0(Q,\omega)}\ . \tag{52}$$

The same manipulations as for the LZ theory lead to a prediction for $F_{\rm RPA}(Y)$

$$F_{\rm RPA}(Y)=\frac{F_{\rm IA}(Y)+\pi\Gamma[F^2_{\rm IA}(Y)+G^2_{\rm IA}(Y)]}{[1+\pi\Gamma F_{\rm IA}(Y)]^2+[\pi\Gamma G_{\rm IA}(Y)]^2}\ , \tag{53}$$

where Γ is defined in Eq. (50), and

$$G_{\rm IA}(Y)\equiv\frac{1}{\pi}P\int_{-\infty}^{\infty}d'\frac{F_{\rm IA}(Y')}{Y-Y'}\ . \tag{54}$$

This does not have the form of a convolution, so that an $R_{\rm RPA}(Y)$ cannot be defined. Like HCPT and LZ, RPA broadens the sharp Bose condensate peak in ^{4}He. Also, it has the same Lorentzian wings in the asymptotic limit as the LZ theory; that is

$$\text{large}\ |Y|\quad F_{\rm LZ}(Y)=F_{\rm RPA}(Y)\rightarrow\frac{\Gamma}{\pi Y^2}\ , \tag{55}$$

RPA also does not satisfy the ω^2 sum rule, Eq. (33b). I shall show in Sec. V that a solution of Eq. (29) does satisfy the ω^2 sum rule, so that the Lorentzian wings predicted by both LZ and RPA, Eq. (55), are absent in HCPT. For the asymptotic limit, all three theories (LZ, RPA, and HCPT) predict a Y scaling broadening of the IA.

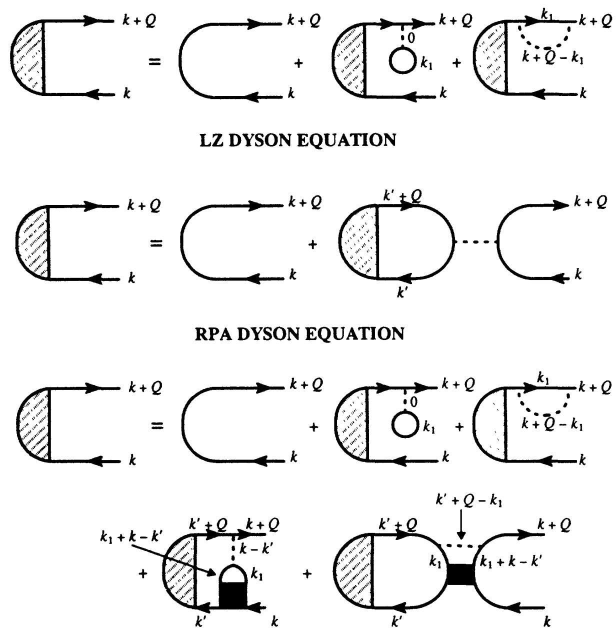

FIG. 3. Diagrammatic representation of the Lorentzian broadening (LZ), t-matrix RPA, and hard core perturbation theory (HCPT) Dyson equations for the $S^Q_k(\omega)$ (hatched) in the high Q limit appropriate to deep inelastic neutron scattering. The filled boxes represent the difference between the two-particle density matrix, Eq. (24), and the $g(r)\rightarrow 1$ limit of the two-particle density matrix, i.e., box$=\Phi_{k_1k_2q}-n_{k_1}n_{k_2}\delta_q$. The lines with right arrows are particle lines. The lines with left arrows are hole lines. The dashed lines represent $T_{k_1k_2q}$.

For helium at finite Q, the three theories predict a slow logarithmic approach to the IA governed by the behavior of $\sigma_{\rm tot}$ at high Q.

A diagrammatic representation of these three theories is shown in Fig. 3. The LZ theory corresponds to only self-energy terms. The RPA corresponds to only summation of bubble diagrams. The HCPT includes self-energy, vertex, and bubble diagram summations, but the "effective" interaction is a product of a $T^B_{k_1k_2q}$ with a $\Phi_{k_1k_2q}$ such that the high-momentum components of the interaction are screened by the ground-state correlations. I note that such screening is the physical idea behind phenomenological polarization potentials for quantum fluids,[42] although a treatment of collective modes with these ideas is beyond the scope of the present paper.

V. SEMICLASSICAL SOLUTION OF THE DYSON EQUATION FOR DINS

In this section, I solve the HCPT Dyson equation, (29), by semiclassical methods within an approximation for the two-particle density matrix, $\Phi_{k_1k_2q}$. The semiclassical methods are extensions of those[43-45] which have been successfully used in the description of He-He scattering.

I show how HCPT satisfies the sum rules for $S(Q,\omega)$. I compare with the quasiclassical theory of Silver and Reiter,[30] the earlier quantum theory by Gersch and Rodriguez,[13] and the Brueckner theory of Weinstein and Negele.[16] I discuss the $O(Q^{-1})$ extensions beyond the asymptotic limit, which are important to the interpretation of reactor neutron experiments.

I begin by simplifying Eq. (29). Because the high Q limit of $T^B_{k_1,k+Q,q}$ is given by Eq. (36), I focus on

$$\frac{1}{n_k}\sum_{k_1}\Phi_{k_1,k,q} \tag{56}$$

which occurs in the sum in Eq. (29). While there have been no full calculations of the two-particle density matrix,[46] the sum rules [Eqs. (25) and (26)] relate $\Phi_{k_1k_2q}$ to n_k, which has been theoretically predicted, and to $g(r)$ which has been both predicted and measured by neutron diffraction experiments. I know the n_k weighted average of (56). Therefore, I replace this quantity by its n_k weighted average over k

$$\frac{1}{n_k}\sum_{k_1}\Phi_{k_1,k,q}\rightarrow\rho\int d^3r\,e^{iqr}g(r)\ . \tag{57}$$

This also satisfies Eq. (26). Note that (57) is true only in an average sense, and it would be interesting to have a correlated basis function evaluation of $\Phi_{k_1k_2q}$ to obtain a more exact theory. With this approximation $S_k^Q(\omega)$ no longer depends on n_k, and therefore a convolution form for the final-state broadening is possible. That is, it will be possible to derive a final-state broadening function for the HCPT theory, $R_{\mathrm{HCPT}}(Y)$.

A solution for $S_k^Q(\omega)$ will be found which depends only on the $k_\parallel$ component of k. First, I rewrite Eq. (29) in more compact form by making the definitions

$$I'(k_\parallel)\equiv\frac{Q}{M}S_k^Q(\omega) \tag{58}$$

and

$$\Gamma'(Q_\parallel)\equiv-\frac{M\rho}{Q}\int\frac{d^2q_\perp}{(2\pi)^2}t(Q/2,2q_\perp/Q)\int d^3r\,e^{i\mathbf{q}\cdot\mathbf{r}}g(r)\ . \tag{59}$$

Then, Eq. (29) looks very simple

$$(Y-k_\parallel)I'(k_\parallel)=i-\int_{-\infty}^{\infty}\frac{dk'_\parallel}{2\pi}\Gamma'(k_\parallel-k'_\parallel)I'(k'_\parallel)\ . \tag{60}$$

This has the form of a convolution, and it may be solved by Fourier transform, i.e.,

$$I(x)\equiv\int_{-\infty}^{\infty}\frac{dk_\parallel}{2\pi}e^{ik_\parallel x}I'(k_\parallel) \tag{61}$$

so that Eq. (60) becomes

$$\left[Y+i\frac{d}{dx}\right]I(x)=i\delta(x)-\Gamma(x)I(x)\ . \tag{62}$$

The solution of Eq. (62) is

$$I(x)=\Theta(x)\exp\left[i\int_0^x dx'[Y+\Gamma(x')]\right]\ , \tag{63}$$

where $\Theta(x)$ is a step function. Then

$$\frac{Q}{M}S^Q_{k_\parallel}(\omega)=\int_0^\infty dx\,\exp\left[i\left[-k_\parallel x+Yx+\int_0^x\Gamma(x')dx'\right]\right]\ . \tag{64}$$

Finally, plugging this into Eqs. (18) and (31), the final-state broadening for HCPT is predicted to be a convolution

$$R_{\mathrm{HCPT}}(Y)=\frac{\mathrm{Re}}{\pi}\int_0^\infty dx\,\exp\left[i\left[Yx+\int_0^x\Gamma(x')dx'\right]\right]\ . \tag{65}$$

Next, I solve for the $\Gamma(x)$ in Eq. (65), which is the Fourier transform of Eq. (59). The scattering angle, Eq. (40), is small and the order of partial waves which contribute is high. Therefore, I can use the small-angle large-l approximation for Legendre polynomials in terms of Bessel functions

$$P_l(\cos\theta)\simeq J_0((l+\tfrac{1}{2})\theta)=\frac{1}{2\pi}\int_0^{2\pi}d\phi\,\exp\left[i\left[l+\frac{1}{2}\right]\frac{2}{Q}\mathbf{q}_\perp\cdot\mathbf{n}(\phi)\right]\ . \tag{66}$$

Equation (66) means that the forward diffractive scattering dominates in Eq. (29). Here, $\mathbf{n}(\phi)$ is a unit vector. Then doing the $d^2q_\perp$ integral in Eq. (59) forces

$$\mathbf{r}_\perp\rightarrow-\left[l+\frac{1}{2}\right]\frac{2}{Q}\mathbf{n}(\phi)\ . \tag{67}$$

I define the impact parameter, b, by

$$b\equiv\left[l+\frac{1}{2}\right]\frac{2}{Q}\ . \tag{68}$$

Then it is straightforward to derive

$$\Gamma(x)=\frac{8\pi\rho}{iQ^2}\sum_{l\text{ even}}(2l+1)(e^{2i\delta}-1)g[(b^2+x^2)^{1/2}]\ . \tag{69}$$

To turn the summation over partial waves in Eq. (69) into an integral over impact parameters, I use the Poisson summation formula

$$\sum_{l\text{ even}}(2l+1)(e^{2i\delta_l}-1)P_l(\cos\theta)=\int_0^\infty dl\,(2l+1)f_lP_l(\cos\theta)\ , \tag{70}$$

where

$$f_l\equiv e^{2i\delta_l}-1+\sum_{\substack{M\text{ even}\\(\neq 0)}}e^{2i\delta_l+iM\pi l}+\sum_{M\text{ odd}}e^{2i\delta_l+iM\pi l}\ . \tag{71}$$

This can be rewritten in terms of b

$$\Gamma_{\mathrm{HCPT}}(x)=\frac{2\pi\rho}{i}\int_0^\infty db\,bf_bg[(b^2+x^2)^{1/2}]\ , \tag{72}$$

where f_b has the obvious definition. This is simply related to the He-He t matrix by

$$\lim_{\substack{x\to\infty \\ \text{or } g(r)\to 1}} \Gamma_{\mathrm{HCPT}}(x) = -\frac{M\rho}{Q} t\left[\frac{Q}{2},0\right]$$
$$\mathrm{Im}\,\Gamma_{\mathrm{HCPT}}(\infty) = \frac{\rho}{2}\sigma_{\mathrm{tot}} \tag{73}$$

according to the optical theorem. So in these limits, the LZ results for the final-state broadening are recovered. However, the $g(r)$ in Eq. (72) screens the scattering at short distances resulting in the prediction of a non-Lorentzian broadening for HCPT.

The HCPT theory, Eqs. (65) and (72), has a very simple physical interpretation. Essentially, it amounts to a classical trajectory calculation for a particle of momentum Q where the effect of scattering is to pick up a complex phase proportional to the t matrix, and where the rate for scattering at position x along the trajectory is proportional to the probability $g[(x^2+b^2)^{1/2}]$ of encountering a particle with impact parameter b. Y has become the conjugate variable to the distance, x, along the trajectory.

In the asymptotic limit, one has

$$\Gamma_{\mathrm{HCPT}}(x) \simeq 2\pi i\rho \int_0^{r_0} db\, b\, g[(b^2+x^2)^{1/2}] \tag{74}$$

which yields Y scaling via Eq. (65). For FSE in He at finite but large Q, one could calculate a Q dependent r_0 which decreases logarithmically with increasing Q. This would appear to be approximate Y scaling apart from the slow logarithmic variation of r_0. Or one could retain the full phase shift analysis which would keep some terms of $O(Q^{-1})$, such as those which give rise to the glory oscillations of the He-He cross section. The $g(r)$ is to a good approximation zero for $r \le r_0$.

Using Eqs. (65) and (74), let us examine the sum rules, Eqs. (32) and (33). Straightforward algebra gives

$$\int_{-\infty}^{\infty} dY\, Y^n R_{\mathrm{HCPT}}(Y) = \lim_{x\to 0} \frac{\mathrm{Re}}{2\pi}\left[i\frac{d}{dx}\right]^n \exp\left[i\int_0^x \Gamma(x')dx'\right] . \tag{75}$$

Invoking the property that $\Gamma(x)$ is an even function of x, the sum rules become

$$f \text{ sum rule}\rightarrow \int_{-\infty}^{\infty} YR_{\mathrm{HCPT}}(Y)dY = -\frac{\mathrm{Re}}{2\pi}\Gamma(0) , \tag{76a}$$

$$\omega^2 \text{ sum rule}\rightarrow \int_{-\infty}^{\infty} Y^2R_{\mathrm{HCPT}}(Y)dY = \frac{\mathrm{Re}}{2\pi}\Gamma^2(0) , \tag{76b}$$

$$\omega^3 \text{ sum rule}\rightarrow \int_{-\infty}^{\infty} Y^3R_{\mathrm{HCPT}}(Y)dY = \frac{\mathrm{Re}}{2\pi}\left[\frac{d^2\Gamma}{dx^2}(0)-\Gamma^3(0)\right] . \tag{76c}$$

But since $g(r)$ is zero for $r \le r_0$ one finds using Eq. (74) that the $\Gamma(0)$, and its second derivative, are zero. The right-hand sides of Eqs. (76) are zero, so that HCPT satisfies all the sum rules.

Qualitatively, small-$|Y|$ corresponds to large x where $\Gamma(x)$ goes to Lorentzian result, Eq. (50). Since the total second moment is zero, at large-$|Y|$ $R_{\mathrm{HCPT}}(Y)$ must be negative. This leads to a suppression of the high-$|Y|$ components of $F(Y)$ compared to $F_{\mathrm{IA}}(Y)$. HCPT qualitatively agrees with the paper of Weinstein and Negele,[16] and it disagrees with Lorentzian broadening theories[9,17–20] which have predicted an enhancement of the high-$|Y|$ components of $F(Y)$. Unfortunately, Weinstein and Negele only treated the high-$|Y|$ behavior of the final-state effects, and they made no predictions for the small-$|Y|$ region which is important to the determination of the Bose condensate fraction in ^{4}He.

It is interesting to compare the HCPT results to the predictions of the two prior theories for FSE which involve $g(r)$. These theories assume that the effective r_0 is the same as the hard-sphere radius which might be obtained by, say, a fit of a Percus-Yevick equation to $g(r)$. In fact, the radius characterizing high-energy collisions is usually significantly smaller than the radius characterizing the spatial structure.

The 1987 quasiclassical (QC) theory of Silver and Reiter[31] produces an integral over a classical trajectory which is almost identical to HCPT

$$R_{\mathrm{QC}}(Y) = \frac{\mathrm{Re}}{\pi}\int_0^{\infty} dx \exp\left[i\left[Yx+\int_0^{x/2}\Gamma_{\mathrm{QC}}(x')dx'\right]\right] . \tag{77}$$

This is the same as Eq. (65) except for the factor of $\frac{1}{2}$ in the limit of the integral. Γ_{QC} is identical to Eq. (74) except that the argument of $g(r)$ is different

$$r^2_{\mathrm{HCPT}} = x^2+b^2, \quad r^2_{\mathrm{QC}} = [x+(r_0^2-b^2)^{1/2}]^2+b^2 . \tag{78}$$

The geometrical interpretation is that r_{HCPT} is the distance between the centers of the two He atoms whereas r_{QC} is the distance between their edges. These theories differ by a factor of 2 in the small Y broadening corresponding to the difference of 2 in the classical and quantum cross sections.

In 1973 Gersch and Rodriguez (GR) derived[15] a result which may be written in terms of Y as

$$R_{\mathrm{GR}}(Y) = \frac{\mathrm{Re}}{\pi}\int_0^{\infty} dx\, e^{iYx-E(x)} , \tag{79}$$

where

$$E(x) = \rho\int d^3r\, \Theta(|\mathbf{r}|-r_0)\Theta(|\mathbf{r}+\mathbf{x}|-r_0)\left[1-\exp\frac{i2M}{Q}\int_0^x dz[V(\mathbf{r}+\mathbf{z})-V(\mathbf{r}+\mathbf{x})]\right] . \tag{80}$$

The term in large parentheses in Eq. (80) is similar to the eikonal approximation[47] for the scattering amplitude. The effect of real space correlations is approximated in the step functions, $\Theta(x)$, which correspond to $g(r) \to \Theta(|r|-r_0)$. Equations (79) and (80) can be put into a form which is almost identical to HCPT by a series of manipulations: (1) at high Q the only nonzero contributions to (80) come from the parts of the integral over $\mathbf{r}$ which make the phase of the second term in brackets oscillate rapidly; (2) identify $r_\perp \to b$ and $r_\parallel \to -x' + (r_0^2-b^2)^{1/2}$; (3) consider $V(r) \simeq V_0\Theta(r_0-|\mathbf{r}|)$ in the limit $V_0 \to \infty$; (4) derive the resulting

$$\Gamma_{\rm GR}(x)=2\pi i\rho\int_0^{r_0} db\, b\Theta[x-2(r_0^2-b^2)^{1/2}] \tag{81}$$

to be used in Eq. (65).

In contrast, within the same step function approximation for $g(r)$ and classical turning point approximation for the phase shifts, one obtains

$$\Gamma_{\rm HCPT}(x)\simeq 2\pi i\rho\int_0^{r_0} db\, b\Theta[x-(r_0^2-b^2)^{1/2}]\ . \tag{82}$$

For completeness, the analogous quasiclassical formula to be used in Eq. (65) is

$$\Gamma_{\rm QC}(x)\simeq \pi i\rho\int_0^{r_0} db\, b\Theta\left[\frac{x}{2}+2(r_0^2-b^2)^{1/2}\right] \tag{83}$$

and the LZ broadening theory is

$$\Gamma_{\rm LZ}(x)\simeq \pi i\rho r_0^2\ . \tag{84}$$

The t matrix RPA cannot be put into the form of Eq. (65).

A geometrical representation of the HCPT, GR, and QC classical trajectories is shown in Fig. 4. Consider the collision of two particles whose initial configuration is shown. The high-momentum particle has a center at point 1 and the low-momentum particle is centered at point 2. The impact parameter for the collision is b. The range of force between the two particles is shown by the circle with radius r_0. Now, imagine particle 1 moving to the right as shown by the arrow. The QC theory considers the collision to have occurred when the point QC passes through 2. The HCPT considers the collision to have occurred when the point labeled HCPT passes through 2. Finally, the GR theory is the same, but for the point labeled GR. Alternatively, the variable x is the distance between point 2 and points QC, HCPT, and GR in the three theories. The high momentum is Q for HCPT and GR, and it is $Q/2$ for QC. I have no explanation for the approximations which led to these differences between the three theories.

The HCPT is certainly more general than the QC and GR theories, as it takes into account the real $g(r)$, uses the real behavior of the He-He phase shifts, has a well developed connection to conventional perturbation theories as discussed in Sec. IV, and has the potential to be extended to $O(Q^{-1})$ phenomena such as the glory oscillations and asymmetry due to the off-energy shell behavior of the t matrix.

There are many terms of $O(Q^{-1})$ which should be dropped in the asymptotic limit, but which will be important for experiments on helium at low to modest Q. While a systematic treatment of such terms is beyond the scope of this paper, it is possible to draw some conclusions from HCPT. Consider first the "hard-sphere glory oscillations" of the final-state broadening which have played an important historical role[26,27] in the development of this subject. The principal contributions to the integral over impact parameters in Eq. (72) come from the stationary phase regions. In the asymptotic limit

$$\lim_{\rm hs}\delta_b \to \delta_b^{\rm HS}=\frac{Q}{2}\left[b\,{\rm acos}\frac{b}{r_0}-(r_0^2-b^2)^{1/2}\right]\ . \tag{85}$$

Equation (85) may be used to show that only the $M=-1$ term in the summations in Eq. (71) has a stationary phase, so to an excellent approximation

$$f_b \to e^{2i\delta_b}-1+e^{2i\delta_b-i\pi Qb/2}\ . \tag{86}$$

Expanding the phase of the third term in Eq. (86) about $b=0$ in the hard-sphere limit

$$2\delta_b-\frac{\pi Qb}{2}\simeq -Qr_0-\frac{Qb^2}{2r_0}\ . \tag{87}$$

Performing the stationary phase integral one obtains for the $M=-1$ term in Eq. (71)

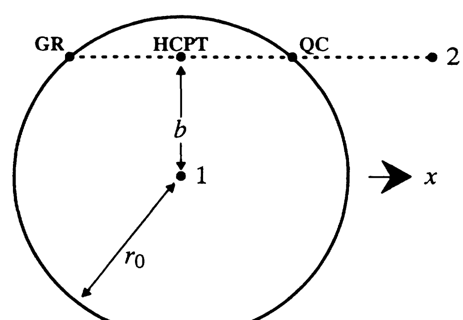

FIG. 4. Schematic representation of the classical trajectories which contribute to hard-core perturbation theory (HCPT), quasiclassical (QC), and Gersch and Rodriguez (GR) theories for final-state effects in DINS. Shown is the initial configuration of particles 1 and 2 immediately after a neutron imparts a high-momentum Q to particle 1. The circle of radius r_0 represents the range of the steeply repulsive core of the potential about particle 1. Particle 1 moves to the right colliding with particle 2 with impact parameter b. The final-state broadening function is the fourier transform of the probability of no collisions as a function of the distance x along the trajectory. The DINS scaling variable, Y, is the conjugate variable to x. The probability of a collision is governed by the radial distribution function, $g(r)$, where r is the distance between particles 1 and 2, $r=(x^2+b^2)^{1/2}$, and x is the distance between particle 2 and the point with the corresponding theory label. In QC the moving particle has momentum $Q/2$.

$$\Gamma_{-1}(\infty) \simeq -\frac{2\pi\rho r_0}{Q} e^{-iQr_0} , \quad (88)$$

Eq. (88) also holds for the He-He potential with r_0 a Q-dependent classical turning point. This term produces the "hard-sphere glory oscillations" in the He-He cross section via Eq. (68), which may be understood in terms of quantum interference between forward and backward scattering.[44] However, the effect of $g[(x^2+b^2)^{1/2}] \rightarrow g(x)$ in the stationary phase integral is to strongly suppress such terms in Eq. (67), so HCPT predicts that glory oscillations in the FSE should be much smaller than in the cross section. In contrast, in the LZ and RPA theories the glory oscillations would be comparable to those of the cross section. The results for ^{3}He are similar in form to Eqs. (67), involving the spin up-up and spin up-down $g(r)$. The results are identical in the approximation that these $g(r)$ are the same, except that the third term in Eq. (83) is multiplied by a $-\frac{1}{2}$ for Fermi statistics.

Other terms which are $O(Q^{-1})$ include: The large impact parameter behavior of the phase shifts which involves the attractive part of the potential; the off-energy-shell behavior of the t matrix;[15] the e_k in Eq. (23); self-energy corrections to the low-momentum particles;[19] etc. A detailed comparison of theory with reactor neutron experiments on ^{4}He and ^{3}He at modest Q's should include all these effects which are not important in the asymptotic limit considered in the present paper.

VI. CONCLUSIONS AND DISCUSSION

The primary conclusion of this paper is that in DINS experiments the impulse approximation to the scattering law should be convoluted with a final state broadening function, $R_{\mathrm{HCPT}}(Y)$. This is expressed in terms of the radial distribution function, $g(r)$, and the He-He phase shifts by Eqs. (65), (72), and (86), which are reproduced below to summarize the results of this paper

$$R_{\mathrm{HCPT}}(Y) = \frac{\mathrm{Re}}{\pi} \int_0^\infty dx \exp\left[i \left[Yx + \int_0^x \Gamma(x')dx' \right] \right] \quad (65)$$

$$\Gamma_{\mathrm{HCPT}}(x) = \frac{2\pi\rho}{i} \int_0^\infty db\, b f_b g[(b^2+x^2)^{1/2}] , \quad (72)$$

$$f_b \rightarrow e^{2i\delta_b} - 1 + e^{2i\delta_b - \pi Q b/2} \quad (86)$$

$R_{\mathrm{HCPT}}(Y)$ is relatively easy to calculate and apply. It satisfies the relevant sum rules including the f sum rule, the ω^2 sum rule, and the ω^3 sum rule. To satisfy the ω^2 sum rule it must be non-Lorentzian. In the asymptotic limit of infinite Q and a hard-core short-range potential, the theory provides a Y scaling correction to the IA. For the helium potential which is exponentially repulsive at short distances, the final-state broadening of the IA plotted on a Y scale decreases slowly as $\ln Q$ at large but finite Q. I have provided a review of the predictions of most of the prior theories of DINS experiments,[9,15-24] and I have shown how most of them can be obtained as approximations to the present hard core perturbation theory (HCPT).

The many-body formalism of HCPT involves Liouville perturbation theory and projection superoperator methods which have previously been applied to diagonal singularity resummations in transport theory.[32-34] The extension to off-diagonal singularities has permitted the development of a perturbation theory for the neutron scattering law for strongly correlated ground states. The dynamical response has been calculated using ground-state properties such as $g(r)$ and n_k obtained by experiment or other many-body theory. The result was a perturbation expansion in which the high-momentum (hard-core) components of the interaction were screened by the ground-state spatial correlations, as one physically expects. I believe that such methods should be applicable to a variety of other problems involving strongly correlated ground states.

In the high Q limit, HCPT has been shown to be equivalent to a classical trajectory calculation. However, this trajectory differed from both Wigner's quasiclassical method[31] and Gersch and Rodriguez's[15] application of the eikonal approximation. These differing semiclassical approximations deserve further exploration in their own right.

Numerical predictions[2] and a comparison with DINS experiments[3] for superfluid ^{4}He at pulsed neutron sources[48] will be presented in following papers.

ACKNOWLEDGMENTS

Special thanks to J. W. Clark for his advice and encouragement throughout the course of this project. I also thank K. Bedell, G. Reiter, and P. Sokol for many helpful discussions. I thank P. Lomdahl for assistance with computations. Los Alamos Neutron Scattering Center (LANSCE) funding provided by the Office of Basic Energy Sciences, Division of Materials Science of the U. S. Department of Energy.

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