Dynamic many-body theory: Pair fluctuations in bulk ^{4}He

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Dynamical excitations in bulk liquid ^{4}He are investigated by using a manifestly microscopic theory of excitations that includes multiple-phonon scattering. The wave function of the dynamic system is represented in terms of one- and two-body excitation amplitudes. Equations of motion for the linear response of boson liquids to a scalar external field are then derived from a stationarity principle. For a consistent treatment of long- and short-wavelength properties of the excitation amplitudes we derive and solve three sets of generic "hypernetted chain" equations determining the basic ingredients of the theory. From those ingredients, we calculate a dynamic structure function for ^{4}He at saturation density. It is shown that the complete solution of the hypernetted chain equations leads, partly by the cancellation of errors, to an insignificantly improved theoretical prediction for the dynamic structure function compared with approximations introduced by Jackson, Feenberg, and Campbell. The implications of this result and the need for including higher-order multiparticle fluctuations are discussed.

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I. INTRODUCTION

The microscopic description of a strongly interacting system conventionally starts with an empirical Hamiltonian

$$H_0 = \sum_{i=1}^{N} \left\{ -\frac{\hbar^2}{2m}\nabla_i^2 + U_{ext}(\mathbf{r}_i) \right\} + \sum_{1\le i<j\le N} v(|\mathbf{r}_i - \mathbf{r}_j|), \tag{1.1}$$

where $U_{ext}(\mathbf{r})$ is an external potential and $v(|\mathbf{r}_i-\mathbf{r}_j|)$ is the interaction between individual particles. Variational methods have been developed over the past three decades to a level where the quantitative prediction of ground-state properties of bulk Bose liquids is a routine matter. The ground-state wave function for a system of N identical bosons with coordinates $\mathbf{r}_1,\ldots,\mathbf{r}_N$ is written in the variational Feenberg form[1]

$$\Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \exp\frac{1}{2}\left\{ \sum_i u_1(\mathbf{r}_i) + \sum_{i<j} u_2(\mathbf{r}_i,\mathbf{r}_j) + \sum_{i<j<k} u_3(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k) + \cdots \right\}. \tag{1.2}$$

The one-body function $u_1(\mathbf{r})$ determines the spatial structure of the system and the two-body function $u_2(\mathbf{r}_i,\mathbf{r}_j)$ describes the short- and long-range correlations between pairs of particles. Triplet correlations are needed to provide quantitative agreement between theoretical predictions and the experimental equation of state,[2–4] and contribute visibly to the nearest-neighbor peak of the pair-distribution function. The correlation functions $u_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)$ are determined by minimization of the energy-expectation value E_0,[2,5]

$$\frac{\delta E_0}{\delta u_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)} = 0. \tag{1.3}$$

Besides simulation methods, the "hypernetted chain" (HNC) hierarchy of integral equations has proven to be a robust method that can reproduce, with minimal phenomenological input, the equation of state of a wide variety of systems. Ingredients are two- and three-body correlations that are optimized by the appropriate Euler-Lagrange (EL) Eq. (1.3). The solution of the full nonlinear HNC equations is necessary for a meaningful optimization of the pair correlations (HNC-EL equations). On the other hand, a specific approximate treatment of the triplet correlations[2,3] dubbed "uniform limit" or "convolution approximation" (CA) has turned out to be sufficient.[3,4]

If a small time-dependent perturbation

$$\delta H(t) = \sum_i \delta U_{\rm ext}(\mathbf{r}_i;t) \tag{1.4}$$

momentarily drives the system out of its ground state, the Jastrow-Feenberg variational wave function, Eq. (1.2), will become time dependent. The logical extension of the ground-state theory is then to write the perturbed wave function as

$$|\Psi(t)\rangle = \frac{e^{-iE_0t/\hbar}e^{\delta U(t)/2}|\Psi_0\rangle}{[\langle\Psi_0|e^{\mathcal{R}e\,\delta U(t)}|\Psi_0\rangle]^{1/2}}, \tag{1.5}$$

where $|\Psi_0\rangle$ is the ground-state wave function, E_0 is the corresponding energy, and

$$\delta U(t) = \sum_i \delta u_1(\mathbf{r}_i;t) + \sum_{i<j} \delta u_2(\mathbf{r}_i,\mathbf{r}_j;t) + \cdots \tag{1.6}$$

is the complex *excitation operator.*

The time-dependent parts of the correlations, $\delta u_n(\mathbf{r}_1,\ldots,\mathbf{r}_n;t)$, are determined by an action principle[6,7]

$$\delta\mathcal{S} = \delta\int dt\mathcal{L}(t) = \delta\int dt\langle\Psi(t)|H_0 + \delta H(t) - i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = 0. \tag{1.7}$$

We assume that the external scalar perturbation $\delta H(t)$ is sufficiently small to permit a linearization of the equations of motion in terms of the $\delta u_n(\mathbf{r}_1,\ldots,\mathbf{r}_n;t)$; we can then expand the Lagrangian to second order in $\delta U(t)$. The derivation can be found in numerous places[8–10] and does not need to be

repeated here. The Lagrangian is, to second order in the fluctuations,

$$\mathcal{L}(t) = \frac{1}{8\mathcal{N}}\langle\Psi_0|[\delta U^*(t),[T,\delta U(t)]]|\Psi_0\rangle$$
$$- \frac{i\hbar}{8\mathcal{N}}\langle\Psi_0|\delta\dot{U}(t)\delta U^*(t) - \delta\dot{U}^*(t)\delta U(t)|\Psi_0\rangle$$
$$+ \frac{1}{2\mathcal{N}}\langle\Psi_0|\delta U^*(t)\delta H(t) + \delta H(t)\delta U(t)|\Psi_0\rangle$$
$$\equiv \mathcal{L}_{\text{int}}(t) + \mathcal{L}_t(t) + \mathcal{L}_{\text{ext}}(t), \tag{1.8}$$

where T is the kinetic-energy operator, and it is assumed, without loss of generality, that the fluctuating part of the wave function is orthogonal to the ground state, $\langle\Psi_0|\delta U(t)|\Psi_0\rangle=0$, and $\mathcal{N}=\int d^3r_1\ldots d^3r_N|\Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2$ is the normalization integral of the ground-state wave function, Eq. (1.2).

To rationalize why a full HNC evaluation of the ingredients of the equations of motion should be done, recall the argument for why pair fluctuations have been introduced in the first place: when the wavelength of an excitation becomes comparable to the interparticle distance, it is expected that the *short-ranged* structure of the wave function is affected. The simplest approximation of the excitation operator, $\delta u_n=0$ for $n\geq 2$—we shall refer to this as the "Feynman approximation" because it is identical to that of the original Feynman theory of excitations in liquid ^{4}He (Ref. 11)—does not have this flexibility, therefore the roton energy predicted by the Feynman theory is more than a factor of 2 too high.

The resulting equations of motion including pair fluctuations have mostly been solved at a relatively primitive level, namely, in the aforementioned CA. This approximation leads to an expression for the self-energy that is identical to the one derived in 1960s by correlated Brillouin-Wigner (BW) perturbation theory.[12–15] It is sufficiently simple that it can also be implemented for nonuniform geometries.[8,16]

The apparently so far best implementation of the equations of motion method is due to Saarela and coworkers[9,17,18] who arrived at a rather impressive agreement between theory and experiments. It was, therefore, believed that the truncation of the excitation operator, Eq. (1.6), at the pair fluctuation level is sufficient for a quantitatively accurate description of the dynamics of ^{4}He, and discrepancies between theory and experiment had been due to inadequacies of the CA. Doubts arose when the dynamic theory of single impurities was developed up to the level of time-dependent *triplet* correlations;[19] that extension was necessary to describe the coupling of an impurity to the roton at the right energy. It turned out that the corrections from triplet fluctuations to the CA were formally quite plausible and quantitatively sizeable. It is therefore expected that corrections of similar size originating from triplet fluctuations should arise in the bulk fluid, which implies that the results of Refs. 17 and 18 were closer to experiments than a theory with only pair fluctuations should predict.

The purpose of this work is to bring the implementation of the equations of motion method to the same level as the ground-state theory in the following sense: for the ground-state theory it is known that the *minimum* approximation for the energy that allows for a meaningful optimization of the pair correlations is the hypernetted chain approximation. This approximation is, in the language of perturbation theory, equivalent to the self-consistent summation of ring and ladder diagrams, i.e., the class of "parquet" diagrams.[20–22] We will see that the same set of diagrams is also the minimal set that is needed for a correct treatment of both short- and long-ranged properties of the n-body distribution functions that enter the excitation theory. These properties are that the distribution functions should go to zero when two particles get closer than the range of the hard core and the sequential relations between different order distribution functions. In the implementations of the pair-excitation theory used so far, the above-mentioned short-distance properties were violated.

Our paper is organized as follows: in Sec. II, we will formulate the exact equations of motion for the one- and two-body excitation amplitudes and manipulate these equations to a form that is suitable for numerical implementation. This derivation deviates from that of Ref. 8 in a number of important points. One is that we will introduce, already at the stage of the Lagrangian Eq. (1.8), a set of new functional variables. This might seem cosmetic here, but it will turn out to be an essential step when we include, in future work,[23] triplet fluctuations. The second aspect is a factorization which lets us identify, in analogy to the impurity theory,[24] a "renormalized" form of the self-energy.

The results of Sec. II are formulated entirely in terms of many-body distribution functions and make no assumptions about how these have been obtained. Thus, the ingredients of the theory could also be obtained from simulation results if these should become available with sufficient accuracy.

Section III carries out a diagrammatic analysis of these distribution functions in terms of Abé diagrams in order to determine the minimum set of diagrams that need to be included to have a fully consistent theory. We will show that these are given by an infinite series. The required sets of diagrams are generated by linear equations, i.e., the calculation is easier than a HNC summation.

All of the derivations of Secs. II and III will be formulated for inhomogeneous systems. In homogeneous systems, it is popular to work in momentum space, although the diagrammatic rules are topologically less intuitive. Section II D will therefore specifically formulate the equations of motion derived in Sec. II for a translationally invariant system.

Section IV will finally turn to the numerical implementation of the equations of motion method. Taking ingredients computed with the integral equations derived in Sec. III, we will present results for the dynamic structure function of ^{4}He close to saturation density. Surprisingly, the final result of the pair-excitation version of the equations of motion method is practically indistinguishable from the convolution approximation result. This is, however, consistent with the expected results when triplet fluctuations will be included. The result is, of course also quite satisfactory because it provides a rigorous justification for the relatively simple convolution approximation that has been used in the past.

II. STATIONARITY PRINCIPLE AND THE GENERIC EQUATIONS OF MOTION

We formulate in this section the generic equations of motion for an excitation operator of the form (1.6) in the specific case that the series is truncated at the two-body level. The equations of motion will be given entirely in terms of n-body distribution functions. The essence of this section is largely contained in Ref. 8, but the derivation will be carried out in a different order; the rationale for this will become apparent in future work where we generalize the method to triplet fluctuations.[23] Also, we shall formulate the equations for the case of nonuniform systems. Since we will need three- and four-body distribution functions, there is little technical advantage in the assumption of translational invariance and isotropy.

Central quantities for the further developments are n-body densities

$$\rho_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)=\frac{N!}{(N-n)!}\frac{\int d^3r_{n+1}\ldots d^3r_N|\Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2}{\int d^3r_1\ldots d^3r_N|\Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2} \tag{2.1}$$

and the corresponding n-body distribution functions

$$g_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)=\frac{\rho_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)}{\rho_1(\mathbf{r}_1)\ldots\rho_1(\mathbf{r}_n)}. \tag{2.2}$$

These satisfy the short-ranged properties

$$g_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)=0 \quad \text{if } |\mathbf{r}_i-\mathbf{r}_j|<r_c,$$

where r_c is the hard-core radius of the interaction, and also satisfy the *sequential relations*

$$\int d^3r_n\rho_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)=(N-n+1)\rho_n(\mathbf{r}_1,\ldots,\mathbf{r}_{n-1}).$$

For convenience, we will use the notation $\int d^3\rho_i \equiv \int \rho_1(\mathbf{r}_i)d^3r_i$ for the density-weighted volume integral. Also, a frequently needed function is

$$h_2(\mathbf{r}_1,\mathbf{r}_2)\equiv g_2(\mathbf{r}_1,\mathbf{r}_2)-1. \tag{2.3}$$

A. Fluctuating densities and distribution functions

The central quantities of linear-response theory are the fluctuations of the n-body densities for the wave function, Eq. (1.5). We define these quantities as *complex functions*; the physical fluctuations are their real parts. We can write these fluctuating densities in terms of variations in ground-state densities with respect to the components of the ground-state wave function, Eq. (1.2). Doing these variations, we always think of the Jastrow-Feenberg amplitudes $u_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)$ as the independent functions. Thus

$$\delta\rho_1(\mathbf{r};t)=\int d^3r_1\frac{\delta\rho_1(\mathbf{r})}{\delta u_1(\mathbf{r}_1)}\delta u_1(\mathbf{r}_1;t)+\int d^3r_1d^3r_2\frac{\delta\rho_1(\mathbf{r})}{\delta u_2(\mathbf{r}_1,\mathbf{r}_2)}\delta u_2(\mathbf{r}_1,\mathbf{r}_2;t). \tag{2.4}$$

Using the symmetry

$$\frac{\delta\rho_1(\mathbf{r})}{\delta u_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)}=\frac{1}{n!}\frac{\delta\rho_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)}{\delta u_1(\mathbf{r})}, \tag{2.5}$$

we can also write Eq. (2.4) as

$$\delta\rho_1(\mathbf{r};t)=\int d^3r_1\frac{\delta\rho_1(\mathbf{r}_1)}{\delta u_1(\mathbf{r})}\delta u_1(\mathbf{r}_1;t)+\frac{1}{2!}\int d^3r_1d^3r_2\frac{\delta\rho_2(\mathbf{r}_1,\mathbf{r}_2)}{\delta u_1(\mathbf{r})}\delta u_2(\mathbf{r}_1,\mathbf{r}_2;t). \tag{2.6}$$

A key step at this point is to define a new one-body variable $\delta v_1(\mathbf{r};t)$ by

$$\delta\rho_1(\mathbf{r};t)\equiv\int d^3r_1\frac{\delta\rho_1(\mathbf{r})}{\delta u_1(\mathbf{r}_1)}\delta v_1(\mathbf{r}_1;t)=\int d^3r_1\frac{\delta\rho_1(\mathbf{r}_1)}{\delta u_1(\mathbf{r})}\delta v_1(\mathbf{r}_1;t), \tag{2.7}$$

where

$$\frac{\delta\rho_1(\mathbf{r})}{\delta u_1(\mathbf{r}_1)}=\rho_1(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}_1)+\rho_2(\mathbf{r},\mathbf{r}_1)-\rho_1(\mathbf{r})\rho_1(\mathbf{r}_1)\equiv\rho_1(\mathbf{r})S(\mathbf{r},\mathbf{r}_1)\rho_1(\mathbf{r}_1) \tag{2.8}$$

is recognized to be related to the real-space representation of the static structure function $S(\mathbf{r}_1,\mathbf{r}_2)$. Note that we deviate here in our convention on density factors slightly from the one used in Ref. 8 and related work.

The relationship between $\delta u_1(\mathbf{r};t)$ and $\delta v_1(\mathbf{r};t)$ is then

$$\delta v_1(\mathbf{r};t)=\delta u_1(\mathbf{r};t)+\frac{1}{2!}\int d^3r'\frac{\delta u_1(\mathbf{r}')}{\delta\rho_1(\mathbf{r})}\times\int d^3r_1d^3r_2\frac{\delta\rho_2(\mathbf{r}_1,\mathbf{r}_2)}{\delta u_1(\mathbf{r}')}\delta u_2(\mathbf{r}_1,\mathbf{r}_2;t)=\delta u_1(\mathbf{r};t)+\frac{1}{2!}\int d^3r_1d^3r_2\frac{\delta\rho_2(\mathbf{r}_1,\mathbf{r}_2)}{\delta\rho_1(\mathbf{r})}\delta u_2(\mathbf{r}_1,\mathbf{r}_2;t). \tag{2.9}$$

Here we need to define what the variation with respect to the one-body density means. This can be done in two ways: if we think of obtaining the distribution functions from a simulation calculation, we can express $\delta\rho_2(\mathbf{r}_1,\mathbf{r}_2)/\delta u_1(\mathbf{r}')$ in terms of two- and three-body densities. The first line of Eq. (2.9) can then be taken as a definition of the second line because the inverse of the static structure function, Eq. (2.8), is known as the direct correlation function.

In this work, we will, however, use diagrammatic methods. *A priori*, we should think of the two-body density and/or pair-distribution function as a diagrammatic expansion in

terms of n-body correlation functions $\exp[u_n(\mathbf{r}_1,\ldots,\mathbf{r}_n)]$. These diagrams contain *articulation points.* Summing all diagrams connected the external points through an articulation point $\mathbf{r}_i$ just gives the one-body density $\rho_1(\mathbf{r}_i)$. We therefore may think of $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$ also as an expansion in terms of the pair (and triplet) correlations $\exp[u_2(\mathbf{r}_i,\mathbf{r}_j)]$ and the one-body density. This is, in fact, how the hypernetted chain equations for nonuniform systems are formulated.[25] The expansion is the same as before, except that it has no articulation points, and the individual point is interpreted as containing a factor $\rho_1(\mathbf{r}_i)$ instead of $e^{u_1(\mathbf{r}_i)}$. The variation with respect to the density is understood to be done on this expansion.

We want to use $\delta v_1(\mathbf{r};t)$ as the independent one-body function, but since there is a one-to-one relationship between $\delta v_1(\mathbf{r};t)$ and $\delta\rho_1(\mathbf{r};t)$ that does not involve the other n-body fluctuations, it is the same as keeping the latter as the independent one-body function. For further reference we also need the fluctuation of the pair-distribution function in these variables

$$\delta\rho_2(\mathbf{r}_1,\mathbf{r}_2;t) = [\delta\rho_1(\mathbf{r}_1;t)\rho_1(\mathbf{r}_2) + \rho_1(\mathbf{r}_1)\delta\rho_1(\mathbf{r}_2;t)]g_2(\mathbf{r}_1,\mathbf{r}_2) + \rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)\delta g_2(\mathbf{r}_1,\mathbf{r}_2;t). \tag{2.10}$$

The time-dependent part of the pair-distribution function $\delta g_2(\mathbf{r}_1,\mathbf{r}_2;t)$ consists of two terms

$$\delta g_2(\mathbf{r}_1,\mathbf{r}_2;t) = \delta_\rho g_2(\mathbf{r}_1,\mathbf{r}_2;t) + \delta_u g_2(\mathbf{r}_1,\mathbf{r}_2;t), \tag{2.11}$$

where

$$\delta_\rho g_2(\mathbf{r}_1,\mathbf{r}_2;t) = \int d^3r_3 \frac{\delta g_2(\mathbf{r}_1,\mathbf{r}_2)}{\delta\rho_1(\mathbf{r}_3)}\delta\rho_1(\mathbf{r}_3;t) \equiv \int d^3r_3 \mathcal{R}(\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2)\delta\rho_1(\mathbf{r}_3;t),$$

$$\delta_u g_2(\mathbf{r}_1,\mathbf{r}_2;t) = \int d^3r_3 d^3r_4 \frac{\delta g_2(\mathbf{r}_1,\mathbf{r}_2)}{\delta u_2(\mathbf{r}_3,\mathbf{r}_4)}\delta u_2(\mathbf{r}_3,\mathbf{r}_4;t) \equiv \int d^3\rho_3 d^3\rho_4 \mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)\delta u_2(\mathbf{r}_3,\mathbf{r}_4;t) \tag{2.12}$$

are the fluctuating parts of the pair-distribution function due to the time dependence of $\delta\rho_1(\mathbf{r}_1;t)$—or equivalently $\delta v_1(\mathbf{r}_1;t)$—and $\delta u_2(\mathbf{r}_i,\mathbf{r}_j;t)$, respectively.

For the one-body equation, we also need the one-body current in terms of both the old and the new variables

$$\mathbf{j}(\mathbf{r};t) = \frac{\hbar}{2mi}\left[\rho_1(\mathbf{r})\nabla_\mathbf{r}\delta u_1(\mathbf{r};t) + \int d^3r_1\rho_2(\mathbf{r},\mathbf{r}_1)\nabla_\mathbf{r}\delta u_2(\mathbf{r},\mathbf{r}_1;t)\right] = \frac{\hbar}{2mi}\rho_1(\mathbf{r})\left[\nabla_\mathbf{r}\delta v_1(\mathbf{r};t) - \frac{1}{2}\int d^3\rho_1 d^3\rho_2 \mathbf{W}(\mathbf{r};\mathbf{r}_1,\mathbf{r}_2)\delta u_2(\mathbf{r}_1,\mathbf{r}_2;t)\right] \equiv \mathbf{j}_F(\mathbf{r};t) + \mathbf{j}_p(\mathbf{r};t), \tag{2.13, 2.14}$$

where

$$\mathbf{W}(\mathbf{r};\mathbf{r}_1,\mathbf{r}_2) = \frac{\delta(\mathbf{r}_1-\mathbf{r})}{\rho_1(\mathbf{r})}\nabla_\mathbf{r}h_2(\mathbf{r},\mathbf{r}_2) + \frac{\delta(\mathbf{r}_2-\mathbf{r})}{\rho_1(\mathbf{r})}\nabla_\mathbf{r}h_2(\mathbf{r}_1,\mathbf{r}) + \nabla_\mathbf{r}\mathcal{R}(\mathbf{r};\mathbf{r}_1,\mathbf{r}_2). \tag{2.15}$$

Equations (2.13) and (2.14) define, in an obvious decomposition, a "Feynman current" $\mathbf{j}_F(\mathbf{r};t)$ and a "pair-induced current" $\mathbf{j}_p(\mathbf{r};t)$. The name Feynman current indicates that this term survives in Feynman approximation $\delta u_2(\mathbf{r}_1,\mathbf{r}_2;t)=0$. Note that we have, again, defined $\mathbf{j}_F(\mathbf{r};t)$ and $\mathbf{j}_p(\mathbf{r};t)$ as *complex* quantities.

B. Lagrangian

We now bring the Lagrangian Eq. (1.8) into a form suitable for deriving the equations of motion. Here we deviate from the previous derivation[8] which performed a variation with respect to the $\delta u_n(\mathbf{r}_1,\ldots,\mathbf{r}_n;t)$. This led to a pair of equations of motion that still had to be manipulated to provide independent equations for the one- and two-body fluctuations. Instead, we transform first to the new set of functions $\delta v_1(\mathbf{r};t)$ and $\delta v_2(\mathbf{r},\mathbf{r}';t)\equiv\delta u_2(\mathbf{r},\mathbf{r}';t)$ which leads to a more compact Lagrangian and directly to independent equation of motion. While the procedure is somewhat cosmetic at the level of implementation of the theory presented here, it is an essential step when fluctuating triplets are included.[19,23]

The external field term depends, to first order in the new variables, only on the one-body amplitude $\delta v_1(\mathbf{r};t)$, cf. Eq. (2.7),

$$\mathcal{L}_{\text{ext}}(t) = \mathcal{R}e\int d^3r\delta\rho_1(\mathbf{r};t)\delta U_{\text{ext}}(\mathbf{r};t) = \mathcal{R}e\int d^3\rho_1 d^3\rho_2 \delta U_{\text{ext}}(\mathbf{r}_1;t)S(\mathbf{r}_1,\mathbf{r}_2)\delta v_1(\mathbf{r}_2;t). \tag{2.16}$$

The time-derivative term is conveniently expressed in terms of (time derivatives of) the time-dependent one- and two-body densities $\delta\rho_1(\mathbf{r};t)$ and $\delta\rho_2(\mathbf{r}_i,\mathbf{r}_j;t)$ to be taken to second order in the fluctuations

$$\mathcal{L}_t(t) = -\frac{i\hbar}{8\mathcal{N}}\langle\Psi_0|\delta\dot{U}(t)\delta U^*(t) - \delta\dot{U}^*(t)\delta U(t)|\Psi_0\rangle = -\frac{i\hbar}{8}\left[\int d^3r\dot{\rho}_1(\mathbf{r};t)\delta u_1^*(\mathbf{r};t) + \frac{1}{2}\int d^3r_1 d^3r_2\dot{\rho}_2(\mathbf{r}_1,\mathbf{r}_2;t)\delta u_2^*(\mathbf{r}_1,\mathbf{r}_2;t) - \text{c.c.}\right] = -\frac{i\hbar}{8}\left[\int d^3r\dot{\rho}_1(\mathbf{r};t)\delta v_1^*(\mathbf{r};t) + \frac{1}{2}\int d^3\rho_1 d^3\rho_2\delta_u\dot{g}_2(\mathbf{r}_1,\mathbf{r}_2;t)\delta v_2^*(\mathbf{r}_1,\mathbf{r}_2;t) - \text{c.c.}\right]. \tag{2.17}$$

Inserting the explicit form of our time-dependent correlations allows us to rewrite the interaction term, Eq. (2.18), in terms of one-, two-, and three-body distribution functions,

$$\begin{aligned}\mathcal{L}_{\rm int}(t) &= \frac{\hbar^2}{8m}\Bigg\{\int d^3\rho_1|\nabla\delta u_1(\mathbf{r}_1;t)|^2 + \int d^3\rho_1 d^3\rho_2 g_2(\mathbf{r}_1,\mathbf{r}_2)[\nabla_1\delta u_1(\mathbf{r}_1;t)\cdot\nabla_1\delta u_2^*(\mathbf{r}_1,\mathbf{r}_2;t) + \text{c.c.} + |\nabla_1\delta u_2(\mathbf{r}_1,\mathbf{r}_2;t)|^2] \\ &\quad + \int d^3\rho_1 d^3\rho_2 d^3\rho_3 g_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\nabla_1\delta u_2(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1\delta u_2^*(\mathbf{r}_1,\mathbf{r}_3)\Bigg\} \\ &= \frac{\hbar^2}{8m}\Bigg\{\int d^3\rho_1\left|\nabla_1\delta u_1(\mathbf{r}_1;t) + \int d^3\rho_2 g_2(\mathbf{r}_1,\mathbf{r}_2)\nabla_1\delta u_2(\mathbf{r}_1,\mathbf{r}_2)\right|^2 + \int d^3\rho_1 d^3\rho_2 g_2(\mathbf{r}_1,\mathbf{r}_2)|\nabla_1\delta u_2(\mathbf{r}_1,\mathbf{r}_2;t)|^2 \\ &\quad + \int d^3\rho_1 d^3\rho_2 d^3\rho_3[g_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) - g_2(\mathbf{r}_1,\mathbf{r}_2)g_2(\mathbf{r}_1,\mathbf{r}_3)]\nabla_1\delta u_2(\mathbf{r}_1,\mathbf{r}_2)\cdot\nabla_1\delta u_2^*(\mathbf{r}_1,\mathbf{r}_3)\Bigg\} \\ &= \frac{m}{2}\int d^3\rho_1|\mathbf{v}(\mathbf{r}_1;t)|^2 + \frac{\hbar^2}{8m}\int d^3\rho_1 d^3\rho_2 d^3\rho_3\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)\nabla_1\delta v_2(\mathbf{r}_1,\mathbf{r}_2)\nabla_1\delta v_2^*(\mathbf{r}_1,\mathbf{r}_3),\end{aligned} \tag{2.18}$$

where

$$\mathbf{v}(\mathbf{r};t) = \frac{\mathbf{j}(\mathbf{r};t)}{\rho_1(\mathbf{r})} \tag{2.19}$$

is the local velocity field and we have defined, for further reference,

$$\begin{aligned}\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) &= g_2(\mathbf{r}_1,\mathbf{r}_2)\frac{\delta(\mathbf{r}_2-\mathbf{r}_3)}{\rho_1(\mathbf{r}_2)} + g_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \\ &\quad - g_2(\mathbf{r}_1,\mathbf{r}_2)g_2(\mathbf{r}_1,\mathbf{r}_3).\end{aligned} \tag{2.20}$$

C. Equations of motion

We are now ready to derive the equations of motion for the Lagrangian Eqs. (2.16)–(2.18). The external field term depends only on $\delta v_1(\mathbf{r};t)$, hence

$$\frac{\delta\mathcal{L}_{\rm ext}(t)}{\delta v_1^*(\mathbf{r};t)} = \frac{1}{2}\rho_1(\mathbf{r})\int d^3\rho' S(\mathbf{r},\mathbf{r}')\delta U_{\rm ext}(\mathbf{r}',t),$$

$$\frac{\delta\mathcal{L}_{\rm ext}(t)}{\delta v_2^*(\mathbf{r},\mathbf{r}';t)} = 0 \tag{2.21}$$

as well as

$$\frac{\delta\mathcal{L}_t(t)}{\delta v_1^*(\mathbf{r}_1;t)} = -\frac{i\hbar}{4}\delta\dot\rho_1(\mathbf{r}_1;t),$$

$$\frac{\delta\mathcal{L}_t(t)}{\delta v_2^*(\mathbf{r}_1,\mathbf{r}_2;t)} = -\frac{i\hbar}{8}\rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)\delta_u\dot g_2(\mathbf{r}_1,\mathbf{r}_2;t). \tag{2.22}$$

The interaction term $\mathcal{L}_{\rm int}(t)$ depends on the one-body variable only through the current, hence

$$\frac{\delta\mathcal{L}_{\rm int}(t)}{\delta v_1^*(\mathbf{r};t)} = -\frac{i\hbar}{4}\nabla\cdot\mathbf{j}(\mathbf{r};t). \tag{2.23}$$

Thus, the one-body equation is simply the continuity equation

$$\nabla\cdot\mathbf{j}(\mathbf{r};t) + \dot\rho_1(\mathbf{r};t) = \frac{2}{i\hbar}\rho_1(\mathbf{r})\int d^3\rho' S(\mathbf{r},\mathbf{r}')\delta U_{\rm ext}(\mathbf{r}';t). \tag{2.24}$$

This result has been obtained earlier, see Refs. 8–10. The advantage of the present formulation is that the two-body equation also comes out more directly. In particular, it is immediately obvious that the two-body equation does not contain the external field.

$$\begin{aligned}&-\left\{\frac{\hbar^2}{2m}\frac{1}{\rho_1(\mathbf{r}_1)}\nabla_1\cdot\left[\rho_1(\mathbf{r}_1)\int d^3\rho_3\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)\nabla_1\delta v_2(\mathbf{r}_1,\mathbf{r}_3;t)\right] + \text{same for } 1\leftrightarrow 2\right\} \\ &\quad = i\hbar\delta_u\dot g_2(\mathbf{r}_1,\mathbf{r}_2;t) + i\hbar\int d^3r_3\mathbf{j}(\mathbf{r}_3;t)\cdot\mathbf{W}(\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2).\end{aligned} \tag{2.25}$$

At this point, we go from the time-dependent formulation to frequency space. We make the standard decomposition

$$U_{\text{ext}}(\mathbf{r};t) = U_{\text{ext}}(\mathbf{r})[e^{i\omega t} + e^{-i\omega t}],$$

$$\delta v_n(\mathbf{r}_1, \ldots, \mathbf{r}_n;t) = \delta v_n^{(+)}(\mathbf{r}_1, \ldots, \mathbf{r}_n)e^{-i\omega t} + \delta v_n^{(-)}(\mathbf{r}_1, \ldots, \mathbf{r}_n)e^{i\omega t},$$

$$\delta\rho_1(\mathbf{r};t) = \delta\rho_1^{(+)}(\mathbf{r})e^{-i\omega t} + \delta\rho_1^{(-)}(\mathbf{r})e^{i\omega t},$$

$$\mathbf{j}(\mathbf{r};t) = \mathbf{j}^{(+)}(\mathbf{r})e^{-i\omega t} + \mathbf{j}^{(-)}(\mathbf{r})e^{i\omega t}. \tag{2.26}$$

The pair fluctuations are functions of one frequency only because the pair equations with positive and negative frequency decouple; only the one-body equation will give us eventually a superposition of positive and negative frequencies. Introduce the operators

$$\begin{aligned}\mathcal{E}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2';\hbar\omega) &= -\frac{\hbar^2}{2m}\frac{1}{\rho_1(\mathbf{r}_1)}\nabla_1\cdot[\delta(\mathbf{r}_1-\mathbf{r}_1')\rho_1(\mathbf{r}_1')\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_2')] \\ &\times\nabla_1'\frac{1}{\rho_1(\mathbf{r}_1')} + \text{same for } \{1,1'\}\leftrightarrow\{2,2'\} \\ &-\hbar\omega\mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2') \\ &\equiv \mathcal{T}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2') - \hbar\omega\mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2')\end{aligned} \tag{2.27}$$

such that the pair equation is

$$\int d^3r_1'd^3r_2'\mathcal{E}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2';\pm\hbar\omega)\rho_1(\mathbf{r}_1')\rho_1(\mathbf{r}_2')\delta v_2^{(\pm)}(\mathbf{r}_1',\mathbf{r}_2') = i\hbar\int d^3r_3\mathbf{W}(\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2)\cdot\mathbf{j}^{(\pm)}(\mathbf{r}_3) \tag{2.28}$$

and the pair-induced current becomes

$$\mathbf{j}_p^{(\pm)}(\mathbf{r}) = -\frac{\hbar}{4mi}\rho_1(\mathbf{r})\int d^3\rho_1 d^3\rho_2\mathbf{W}(\mathbf{r};\mathbf{r}_1,\mathbf{r}_2)\delta v_2^{(\pm)}(\mathbf{r}_1,\mathbf{r}_2). \tag{2.29}$$

Equations (2.24) and (2.28) form, together with the connections, Eqs. (2.8) and (2.13), and Eq. (2.29), between the amplitudes, the current, and the density fluctuation, the generic set of equations of motion for the pair fluctuations; see, for example, Appendix A of Ref. 8. Typically, approximations are made at this point to make further progress. Most popular is the uniform limit or convolution approximation in which the operator $\mathcal{E}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2';\omega)$ becomes diagonal in momentum space or, in a nonuniform system, in the space spanned by the Feynman excitations.[8] This approximation is also obtained by second-order Brillouin Wigner perturbation theory.[12,26] Less transparent is the relationship to the work of Saarela[9] who introduces the left-hand side of Eq. (2.11) as the independent two-body quantity and arrives, therefore, at algebraically different equations.

The one- and the two-body equation are still coupled; they can be completely decoupled as follows: define, for any two-point operators $A(\mathbf{r},\mathbf{r}')$ and $B(\mathbf{r},\mathbf{r}')$ the *convolution product*

$$[A*B](\mathbf{r},\mathbf{r}') \equiv \int d^3r''A(\mathbf{r},\mathbf{r}'')\rho_1(\mathbf{r}'')B(\mathbf{r}'',\mathbf{r}') \tag{2.30}$$

as well as the logical extension for a four-point function such as $\mathcal{E}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2';\hbar\omega)$. The *inverse* of an operator A in the sense of the convolution product is

$$[A^{-1}*A](\mathbf{r},\mathbf{r}') \equiv \int d^3r''A^{-1}(\mathbf{r},\mathbf{r}'')\rho_1(\mathbf{r}'')A(\mathbf{r}'',\mathbf{r}') = \frac{\delta(\mathbf{r}-\mathbf{r}')}{\rho_1(\mathbf{r})}, \tag{2.31}$$

and, analogously, for the energy operator

$$\begin{aligned}[\mathcal{E}^{-1}*\mathcal{E}](\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';\omega) &\equiv \int d^3r_3d^3r_4\mathcal{E}^{-1}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4;\hbar\omega) \\ &\times\rho_1(\mathbf{r}_3)\rho_1(\mathbf{r}_4)\mathcal{E}(\mathbf{r}_3,\mathbf{r}_4;\mathbf{r}_1',\mathbf{r}_2';\hbar\omega) \\ &= \frac{\delta(\mathbf{r}_1-\mathbf{r}_1')\delta(\mathbf{r}_2-\mathbf{r}_2')}{\rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)}.\end{aligned} \tag{2.32}$$

We can combine Eqs. (2.28) and (2.29) into

$$\begin{aligned}\mathbf{j}_p^{(\pm)}(\mathbf{r}) &= \mathbf{j}^{(\pm)}(\mathbf{r}) - \mathbf{j}_F^{(\pm)}(\mathbf{r}) \\ &= \rho_1(\mathbf{r})\int d^3r'\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\pm\hbar\omega)\mathbf{j}^{(\pm)}(\mathbf{r}'),\end{aligned} \tag{2.33}$$

where the components of the tensor $\boldsymbol{\sigma}(\mathbf{r},\mathbf{r}';\hbar\omega)$ are defined by

$$\sigma_{ij}(\mathbf{r},\mathbf{r}';\hbar\omega) = -\frac{\hbar^2}{4m}[W_i*\mathcal{E}^{-1}*W_j](\mathbf{r},\mathbf{r}';\omega). \tag{2.34}$$

The total current is then in terms of the Feynman current

$$\mathbf{j}^{(\pm)}(\mathbf{r}) = \rho_1(\mathbf{r})\int d^3r'[\mathbf{1}-\boldsymbol{\sigma}(\pm\hbar\omega)]^{-1}(\mathbf{r},\mathbf{r}')\mathbf{j}_F^{(\pm)}(\mathbf{r}'), \tag{2.35}$$

where

$$\mathbf{1}_{ij}(\mathbf{r},\mathbf{r}') = \delta_{ij}\frac{\delta(\mathbf{r}-\mathbf{r}')}{\rho_1(\mathbf{r})}.$$

We now go back with this solution into the one-body equation and write Eq. (2.24) as

$$\pm\hbar\omega\delta\rho_1^{(\pm)}(\mathbf{r}) + \frac{\hbar^2}{2m}\int d^3r'\{\nabla_{\mathbf{r}}\rho_1(\mathbf{r})[\mathbf{1}-\boldsymbol{\sigma}(\pm\hbar\omega)]^{-1}(\mathbf{r},\mathbf{r}') \times\rho_1(\mathbf{r}')\nabla_{\mathbf{r}'}\}\delta v_1^{(\pm)}(\mathbf{r}') = 2\rho_1(\mathbf{r})\int d^3\rho' S(\mathbf{r},\mathbf{r}')U_{\text{ext}}(\mathbf{r}'). \tag{2.36}$$

Define now a self-energy as

$$\Sigma(\mathbf{r},\mathbf{r}';\hbar\omega) \equiv -\frac{\hbar^2}{2m}\{(S^{-1/2}\nabla) * [\mathbf{1}-\boldsymbol{\sigma}(\hbar\omega)]^{-1} * (\nabla S^{-1/2})\}(\mathbf{r},\mathbf{r}';\hbar\omega) \tag{2.37}$$

and the single-phonon propagator

$$G^{-1}(\mathbf{r},\mathbf{r}';\hbar\omega) \equiv \hbar\omega\frac{\delta(\mathbf{r}-\mathbf{r}')}{\rho_1(\mathbf{r})} + \Sigma(\mathbf{r},\mathbf{r}';\hbar\omega). \tag{2.38}$$

Solving for the real part of the density fluctuations, we finally obtain the coordinate-space representation of the density-density response function

$$\chi(\mathbf{r},\mathbf{r}';\hbar\omega) = \rho_1(\mathbf{r})[S^{1/2} * \{G(\hbar\omega)+G(-\hbar\omega)\} * S^{1/2}](\mathbf{r},\mathbf{r}')\rho_1(\mathbf{r}'). \tag{2.39}$$

This is our final result for this response function; it is identical, in a slightly different notation, to Eq. (2.18) of Ref. 8. We stress, however, again that no approximations have been made so far other than the assumption of pair fluctuations. The appearance of the expression $[\mathbf{1}-\boldsymbol{\sigma}(\hbar\omega)]^{-1}$ is analogous to Owen's "renormalized self-energy" of an impurity in a Bose fluid.[24]

D. Uniform system

In the case of a translationally invariant system and a plane-wave perturbation, the perturbed density can only be a plane wave, and the current a plane-wave current

$$\delta\rho_1(\mathbf{r}) = \rho_0 e^{i\mathbf{q}\cdot\mathbf{r}}, \quad \mathbf{j}(\mathbf{r}) = j_0\rho\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}}. \tag{2.40}$$

Since both the left- and right-hand sides of Eq. (2.33) are in the direction of $\mathbf{q}$, and because of translational invariance, we only need the scalar function

$$\tilde{\sigma}(q,\hbar\omega) \equiv \sum_{ij}\hat{q}_i\sigma_{ij}(q,\hbar\omega)\hat{q}_j, \tag{2.41}$$

where the $\hat{q}_j$ are the components of the unit vector $\hat{\mathbf{q}}$ in the direction of $\mathbf{q}$. Equation (2.33) can then be solved in closed form,

$$\mathbf{j}^{\pm}(\mathbf{r}) = \frac{1}{1-\tilde{\sigma}(q,\pm\hbar\omega)}\mathbf{j}_F^{(\pm)}(\mathbf{r}) \tag{2.42}$$

with $\tilde{\sigma}(q,\hbar\omega)=\rho\int d^3r\sigma(\mathbf{r};\hbar\omega)e^{i\mathbf{q}\cdot\mathbf{r}}$ because $\sigma(\mathbf{r},\mathbf{r}';\hbar\omega)=\sigma(\mathbf{r}-\mathbf{r}';\omega)$ in the homogeneous case. Taking this into the one-body equation gives finally

$$\left[\pm\hbar\omega - \frac{\hbar^2q^2}{2mS(q)}\frac{1}{1-\tilde{\sigma}(q,\hbar\omega)}\right]\rho^{(\pm)}(q) = 2S(q)U_0 \tag{2.43}$$

and leads to the bulk self-energy

$$\Sigma(q,\hbar\omega) = \frac{\varepsilon(q)}{1-\tilde{\sigma}(q,\hbar\omega)} \tag{2.44}$$

and the density-density response function

$$\chi(q,\omega) = \frac{S(q)}{\hbar\omega-\Sigma(q,\hbar\omega)} + \frac{S(q)}{-\hbar\omega-\Sigma(q,-\hbar\omega)}. \tag{2.45}$$

[We deviate here from the previous notation in the sense that we define the Feynman energy $\varepsilon(q)=\hbar^2q^2/2mS(q)$ as a part of the self-energy.]

Previous implementations of the theory have led to a form that is obtained by expanding the term $1/[1-\tilde{\sigma}(q,\hbar\omega)]$ to first order in $\tilde{\sigma}(q,\omega)$. This is obviously not necessary. Following Owen,[24] we shall refer to

$$\Sigma(q,\hbar\omega) = \frac{\varepsilon(q)}{1-\tilde{\sigma}(q,\hbar\omega)} \tag{2.46}$$

as to the renormalized self-energy, whereas the expanded form

$$\Sigma_U(q,\hbar\omega) = \varepsilon(q)[1+\tilde{\sigma}(q,\hbar\omega)] \tag{2.47}$$

will be called the "unrenormalized" form.

For a plane-wave current, Eq. (2.40), we can write the right-hand side of Eq. (2.28) as

$$\begin{aligned} i\hbar\int d^3r_3\mathbf{W}(\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2)\cdot\mathbf{j}(\mathbf{r}_3) &= i\hbar j_0 e^{i\mathbf{q}\cdot\mathbf{R}}\mathbf{q}\cdot[\nabla h_2(r_{12})(e^{i\mathbf{q}\cdot\mathbf{r}_{12}/2}+e^{-i\mathbf{q}\cdot\mathbf{r}_{12}/2}) \\ &\quad + \rho\int d^3r_3 e^{i\mathbf{q}\cdot\mathbf{r}_{32}/2+i\mathbf{q}\cdot\mathbf{r}_{31}/2}\nabla_3\mathcal{R}(\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2)] \\ &\equiv \frac{2m}{\hbar}j_0 e^{i\mathbf{q}\cdot\mathbf{R}}\mathcal{V}^{(3)}(\mathbf{q},\mathbf{r}_{12}), \end{aligned} \tag{2.48}$$

where $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$ and $\mathbf{R}=\frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)$ is the center of mass coordinate. $\mathcal{V}^{(3)}(\mathbf{q},\mathbf{r}_{12})$ is, up to normalization factors, the three-body vertex of correlated BW theory.[12] Equation (2.48) shows that the right-hand side of the pair equation factorizes into a plane wave for the center of mass motion and a translationally invariant term. It is therefore legitimate to take the same form for the pair fluctuation, i.e.,

$$\delta v_2(\mathbf{r}_1,\mathbf{r}_2) = e^{i\mathbf{q}\cdot\mathbf{R}}v_{\mathbf{q}}(\mathbf{r}_{12}). \tag{2.49}$$

With this, we can write the full solution as

$$\sigma(q,\hbar\omega) = \frac{1}{2\varepsilon(q)}\int\frac{d^3p_1d^3p_2}{(2\pi)^6\rho^2}\tilde{\mathcal{V}}^{(3)}(\mathbf{q};\mathbf{p}_1)\tilde{\mathcal{E}}^{-1}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2;\omega) \times\tilde{\mathcal{V}}^{(3)}(\mathbf{q};\mathbf{p}_2). \tag{2.50}$$

Note that this form is completely general for pair fluctuations. In the CA, the energy denominator is diagonal and we obtain the well-known form

$$\sigma^{\mathrm{CA}}(q,\hbar\omega) = \frac{1}{2\varepsilon(q)}\int\frac{d^3p}{(2\pi)^3\rho}\frac{|\tilde{\mathcal{V}}^{(3)}(\mathbf{q};\mathbf{p})|^2}{\hbar\omega-\varepsilon(|\mathbf{q}/2-\mathbf{p}|)-\varepsilon(|\mathbf{q}/2+\mathbf{p}|)}. \tag{2.51}$$

III. DIAGRAMMATIC ANALYSIS

A. Inhomogeneous system

Different implementations of the equations of motion differ, in their essence, in the kind of approximations made depending on the system under consideration. The most frequently used convolution approximation was first derived by Brillouin-Wigner perturbation theory in a correlated basis.[12–15] This approximation amounts, besides the linearization, Eq. (2.47), to the following simplifications

$$\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) \approx \mathcal{F}_{22}^{(\mathrm{CA})}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) = S(\mathbf{r}_2,\mathbf{r}_3),$$

$$\mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) \approx \mathcal{G}_{22}^{(\mathrm{CA})}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = S(\mathbf{r}_1,\mathbf{r}_3)S(\mathbf{r}_2,\mathbf{r}_4),$$

$$\mathcal{R}(\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2) \approx \mathcal{R}^{(\mathrm{CA})}(\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2) = h_2(\mathbf{r}_1,\mathbf{r}_3)h_2(\mathbf{r}_2,\mathbf{r}_3) + u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3), \quad (3.1)$$

where $u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ is the ground-state triplet correlation function. The importance of this contribution has been emphasized by Chang and Campbell.[12]

The CA preserves the long-wavelength features of the equations of motion in the sense that it is the simplest approximation that preserves the convolution identities

$$\int d^3\rho_2 \mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) = 0,$$

$$\int d^3\rho_2 \mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = 0,$$

$$\int d^3\rho_2 \mathcal{R}(\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2) = -h_2(\mathbf{r}_1,\mathbf{r}_3), \quad (3.2)$$

and corresponding relationships generated by symmetry operations. All of these relationships are consequences of the property $\int d^3\rho_2 h_2(\mathbf{r}_1,\mathbf{r}_2) = -1$.

The short-ranged structure of the functions $\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$, $\mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)$, and $\delta g_2(\mathbf{r}_1,\mathbf{r}_2)/\delta\rho_1(\mathbf{r}_3)$ are, on the other hand, violated by the uniform limit approximation. These are

$$\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) \to 0 \quad \text{as} \quad |\mathbf{r}_1-\mathbf{r}_2| \to 0 \quad \text{or} \quad |\mathbf{r}_1-\mathbf{r}_3| \to 0,$$

$$\mathcal{G}_{22}(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) \to 0 \quad \text{as} \quad |\mathbf{r}_1-\mathbf{r}_2| \to 0 \quad \text{or} \quad |\mathbf{r}_3-\mathbf{r}_4| \to 0,$$

$$\mathcal{R}(\mathbf{r}_3;\mathbf{r}_1,\mathbf{r}_2) \to 0 \quad \text{as} \quad |\mathbf{r}_1-\mathbf{r}_2| \to 0. \quad (3.3)$$

There is no simple approximation that satisfies both properties, Eqs. (3.2) and (3.3), and a diagrammatic analysis of what is needed is called for. Figure 1 shows, in the usual diagrammatic language of the HNC theory, the first few diagrams contributing to the three-point function $\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$. Circles indicate "external" points, filled circles indicate a density-weighted volume integration $\int d^3\rho_i$. Solid lines connecting two points $\mathbf{r}_i$ and $\mathbf{r}_j$ represent a function $h_2(\mathbf{r}_i,\mathbf{r}_j)$.

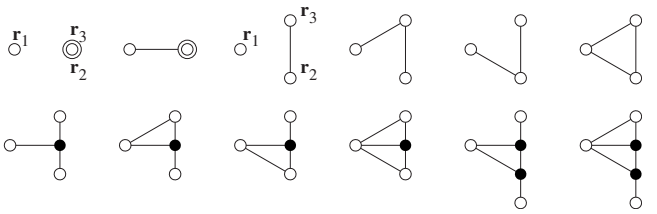

FIG. 1. The figure shows the first few contributions to a diagrammatic expansion of the function $\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$. The coordinates $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ are as shown in the first and the third diagram, the double circle indicates that these coincide, i.e., a factor $\delta(\mathbf{r}_2-\mathbf{r}_3)/\rho_1(\mathbf{r}_2)$.

The short-ranged properties, Eq. (3.3), are seen to emerge as follows: combining diagrams 1 and 2 just gives a function $g_2(\mathbf{r}_1,\mathbf{r}_2)\delta(\mathbf{r}_2-\mathbf{r}_3)/\rho_1(\mathbf{r}_2)$. The sum of the next four diagrams is $g_2(\mathbf{r}_1,\mathbf{r}_2)g_2(\mathbf{r}_1,\mathbf{r}_3)h_2(\mathbf{r}_2,\mathbf{r}_3)$ and therefore satisfies Eq. (3.3). Likewise, the combination of the first four diagrams in the second line leads to a common factor $g_2(\mathbf{r}_1,\mathbf{r}_2)g_2(\mathbf{r}_1,\mathbf{r}_3)$.

The long-wavelength feature, Eq. (3.2), is obtained differently. Carrying out the density-weighted integration over coordinate $\mathbf{r}_2$ leads to the cancellation of diagrams 1 and 3, 2 and 4, 5 and 7, 6 and 8, 9 and 11, as well as 10 and 12. Evidently, different combinations of diagrams are needed to guarantee the properties, Eqs. (3.2) and (3.3), and it takes an infinite series to guarantee both. The uniform limit approximation keeps only the first and the third diagram.

The series of diagrams whose first terms are shown in Fig. 1 can be summed by the usual hypernetted-chain technique, summing "nodal" and "parallel-connected" diagrams self-consistently. Denote, for all three quantities to be calculated, the parallel-connected subset with a superscript X and the nodal subset with a superscript N. Then, the series is summed by the following set of equations,

$$\mathcal{F}_{22}^{(N)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) = \mathcal{F}_{22}^{(\mathrm{CA})}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) + \int d^3\rho_4 \mathcal{F}_{22}^{(X)}(\mathbf{r}_1;\mathbf{r}_4,\mathbf{r}_3)h_2(\mathbf{r}_4,\mathbf{r}_2),$$

$$\mathcal{F}_{22}^{(X)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) = h_2(\mathbf{r}_1,\mathbf{r}_2)\mathcal{F}_{22}^{(N)}(\mathbf{r}_{12},\mathbf{r}_{13}),$$

$$\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) = \mathcal{F}_{22}^{(N)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) + \mathcal{F}_{22}^{(X)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3). \quad (3.4)$$

Similar integral equations for $\mathcal{R}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$ and $\mathcal{G}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)$ are obtained diagrammatically or by variation in the hypernetted chain equations for inhomogeneous systems[25] with respect to $u_2(\mathbf{r}_3,\mathbf{r}_4)$ or $\rho_1(\mathbf{r}_1)$. The first few diagrams contributing to the series are shown in Fig. 2. The same remarks apply about how to group these diagrams such that they have a common factor $g_2(\mathbf{r}_2,\mathbf{r}_3)$ and how to group them such that the sequential relation (3.2) is satisfied.

The integral equation summing these diagrams is

$$\mathcal{R}^{(N)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) = \mathcal{R}^{(\mathrm{CA})}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) + \int d^3\rho_4 \mathcal{R}^{(X)}(\mathbf{r}_1;\mathbf{r}_4,\mathbf{r}_3)h_2(\mathbf{r}_2,\mathbf{r}_4) + \int d^3\rho_5 \mathcal{R}^{(X)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_5)h_2(\mathbf{r}_5,\mathbf{r}_3) + \int d^3\rho_4 d^3\rho_5 \mathcal{R}^{(X)}(\mathbf{r}_1;\mathbf{r}_4,\mathbf{r}_5)h_2(\mathbf{r}_2,\mathbf{r}_4)h_2(\mathbf{r}_3,\mathbf{r}_5),$$

$$\mathcal{R}^{(X)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) = \mathcal{R}^{(N)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)h_2(\mathbf{r}_2,\mathbf{r}_3),$$

$$\mathcal{R}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) = \mathcal{R}^{(X)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3) + \mathcal{R}^{(N)}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3). \quad (3.5)$$

Finally, the integral equation summing the series $\mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)$ is practically identical, only the driving convolution approximation term is different:

$$\mathcal{G}_{22}^{(N)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = \mathcal{G}_{22}^{(\mathrm{CA})}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) + \int d^3\rho_4 \mathcal{G}_{22}^{(X)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_5,\mathbf{r}_4)h_2(\mathbf{r}_3,\mathbf{r}_5) + \int d^3\rho_6 \mathcal{G}_{22}^{(X)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_6)h_2(\mathbf{r}_6,\mathbf{r}_4) + \int d^3\rho_5 d^3\rho_6 \mathcal{G}_{22}^{(X)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_5,\mathbf{r}_6)h_2(\mathbf{r}_3,\mathbf{r}_5)h_2(\mathbf{r}_4,\mathbf{r}_6),$$

$$\mathcal{G}_{22}^{(X)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = \mathcal{G}_{22}^{(N)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)h_2(\mathbf{r}_3,\mathbf{r}_4),$$

$$\mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = \mathcal{G}_{22}^{(X)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) + \mathcal{G}_{22}^{(N)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4). \quad (3.6)$$

The integral equations formulated in Eqs. (3.4)–(3.6) sum only the minimum set of diagrams that is necessary for a consistent treatment of the short- and long-ranged correlations. On the other hand, they are "generic" in the sense that they decompose, for example, the four-point function into sets of diagrams that can be split into two disconnected pieces such that one piece contains the points $\mathbf{r}_1$ and $\mathbf{r}_2$ and the other one the points $\mathbf{r}_3$ and $\mathbf{r}_4$ by cutting them in *two* points. Thus, the rectangle appearing in the last three diagrams of Fig. 2 may be any four-point function that cannot be decomposed as described above. In this interpretation, the series is exact.

It is, of course, also possible to include, without undue computational effort, triplet correlations and elementary diagrams in the diagram summations. Recall that triplet correlations have been found important for understanding the density dependence of the roton minimum;[12] these are therefore routinely included in the convolution approximation, Eq. (3.1). There are, of course, more elementary diagram and triplet corrections to the driving term $\mathcal{R}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$. A few typical diagrams are shown in Fig. 3. The first two diagrams are included in the CA, Eq. (3.1).

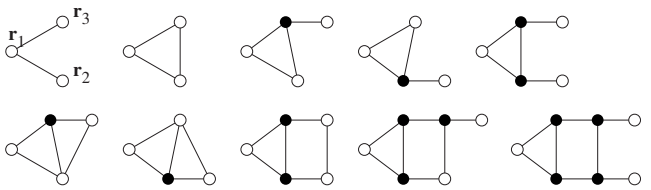

FIG. 2. The figure shows the first few contributions to a diagrammatic expansion of the function $\mathcal{R}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$. The coordinates $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ are as shown in the first diagram. The first diagram shown is the convolution approximation; it should be supplemented with a three-body ground-state correlation $u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ which is not shown here. For elementary diagram and triplet corrections, see Fig. 3.

To test the importance of elementary diagrams and triplet correlations beyond the simplest term, we have calculated the third diagram shown in Fig. 3 as well as all diagrams containing one three-body correlation $u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$. It was found that none of these corrections produced a visible effect on the numerical results; they were therefore not included in production runs.

B. Integral equations for the uniform system

The essential part of the calculation is the solution of the pair Eq. (2.28) or, equivalently, the calculation of the inverse of the energy operator $\mathcal{E}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2';\hbar\omega)$. This looks, at first glance, like a rather formidable problem because the ingredients are, even after using translational invariance and isotropy, still functions of seven variables.

For the uniform system it is convenient to work in momentum space; the necessary manipulations are carried out in Appendices A and B. Define

$$\tilde{\mathcal{G}}_{22}(\mathbf{q};\mathbf{p},\mathbf{p}') = \rho^2 \int d^3r_{12} d^3r_{34} d^3r_{24} e^{-i\mathbf{q}\cdot\mathbf{r}_{24} - i\mathbf{r}_{12}\cdot(\mathbf{p}-\mathbf{q}/2) + i\mathbf{r}_{12}\cdot(\mathbf{p}'-\mathbf{q}/2)} \times \mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) \quad (3.7)$$

and likewise $\tilde{\mathcal{T}}_{22}(\mathbf{q};\mathbf{p},\mathbf{p}')$. We can further expand the angular dependence of the ingredients of the integral kernel $\mathcal{E}(\mathbf{q};\mathbf{p},\mathbf{p}';\omega)$ in Legendre polynomials

$$\tilde{\mathcal{T}}_{22}(\mathbf{q};\mathbf{p},\mathbf{p}') = \sum_{\ell,\ell'} T_{\ell\ell'}(q;p,p')P_\ell(\hat{\mathbf{q}}\cdot\hat{\mathbf{p}})P_{\ell'}(\hat{\mathbf{q}}\cdot\hat{\mathbf{p}}'),$$

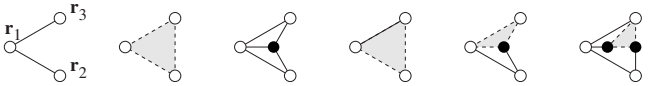

FIG. 3. The figure shows the convolution term in the diagrammatic expansion of the function $\mathcal{R}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$ (leftmost diagram) as well as the triplet correlation $u_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ (gray triangle with dashed borders) that is normally included in the convolution approximation (second diagram). Also shown is the first elementary diagram contribution to $\mathcal{R}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$ (third diagram) as well as a few diagrams containing one three-body function. The coordinates $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ are as shown in the first diagram.

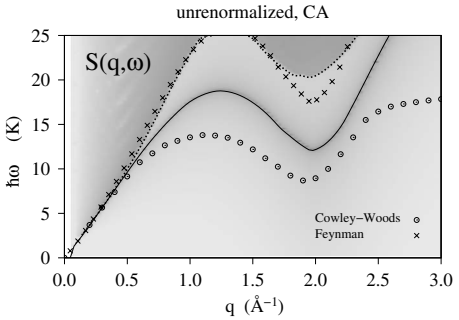

FIG. 4. The figure shows a gray-scale map of the dynamic structure function in convolution approximation for the *unrenormalized* version of the self-energy, Eq. (2.47). Darker values correspond to higher values. The circles are the experimental data of Cowley and Woods (Ref. 29), and the crosses show the Feynman excitation energy $\varepsilon(q)$. The solid line is the dispersion relation of the collective excitation and the dotted line indicates the lowest energy $\hbar\omega_c$ where the self-energy is complex.

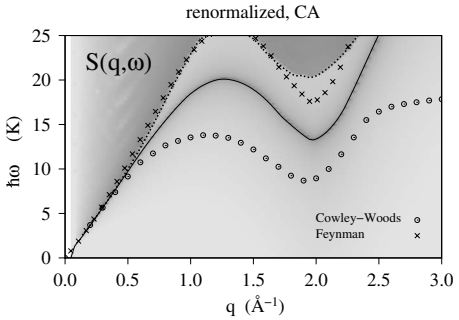

FIG. 5. Same as Fig. 4 for the structure function in convolution approximation for the *renormalized* version of the self-energy, Eq. (2.46).

$$\tilde{\mathcal{G}}_{22}(\mathbf{q};\mathbf{p},\mathbf{p}') = \sum_{\ell,\ell'} G_{\ell\ell'}(q;p,p')P_\ell(\hat{\mathbf{q}}\cdot\hat{\mathbf{p}})P_{\ell'}(\hat{\mathbf{q}}\cdot\hat{\mathbf{p}}'),$$

$$\tilde{\mathcal{E}}(\mathbf{q};\mathbf{p},\mathbf{p};\omega) = \sum_{\ell,\ell'} E_{\ell\ell'}(q;p,p';\omega)P_\ell(\hat{\mathbf{q}}\cdot\hat{\mathbf{p}})P_{\ell'}(\hat{\mathbf{q}}\cdot\hat{\mathbf{p}}'). \tag{3.8}$$

Note that we do not need to expand the integral kernel in terms of spherical harmonics since only the $m=0$ component survives due to the structure, Eq. (B3), of the right-hand side of the equation which implies the form (B4) of the excitation functions. Only even angular momentum components contribute due to the symmetry $\mathbf{q}\leftrightarrow-\mathbf{q}$.

The resulting integral equations in momentum space are spelled out in Eqs. (A2), (A3), and (A5), and the angular momentum decompositions in Eqs. (B6), (B9), and (B11). The angular momentum representation can be solved quite easily, after discretization, either by iteration, or as a system of linear equations. The inverse of $E_{\ell\ell'}(q;p,p';\omega)$ can then be calculated by solving the generalized eigenvalue problem

$$\sum_{\ell'}\int\frac{d^3p'}{(2\pi)^3}T_{\ell\ell'}(q;p,p')v_{\ell'}^{(n)}(p') = \hbar\omega_n\sum_{\ell'}\int\frac{d^3p'}{(2\pi)^3}G_{\ell\ell'}(q;p,p')v_{\ell'}^{(n)}(p'). \tag{3.9}$$

The operator $E^{-1}_{\ell\ell'}(q;p,p';\omega)$ then has the spectral decomposition

$$E^{-1}_{\ell\ell'}(q;p,p';\omega) = \sum_n v_\ell^{(n)}(p)\frac{1}{\hbar\omega_n-\hbar\omega}v_{\ell'}^{(n)}(p'). \tag{3.10}$$

The use of this spectral decomposition is convenient since a small imaginary part needs to be added to the denominator only for those states $v_{\ell'}^{(n)}(p)$ whose energy $\hbar\omega_n$ is close to the target energy $\hbar\omega$. The smallest eigenvalue of Eq. (3.9), referred to here as $\hbar\omega_c$, is the energy below which the self-energy correction is real and, hence, we have a zero-width collective mode. In the convolution approximation, we have

$$\hbar\omega_c^{\mathrm{CA}}(q) = \min_{\mathbf{p}}[\varepsilon(|\mathbf{q}/2-\mathbf{p}|)+\varepsilon(|\mathbf{q}/2+\mathbf{p}|)]. \tag{3.11}$$

IV. RESULTS

We have solved the full pair equations of motion at the HNC level for ^{4}He at a density of $\rho=0.022$ Å^{-3} which is close to the experimental saturation density. We have used the Aziz-II potential[27] for the bare interaction. Input data were generated by HNC-EL calculations described, for example, in Ref. 28, including triplet correlations and scaled elementary diagrams. We have included a gentle modification of the very long-wavelength part of the Feynman spectrum that has the purpose of generating numerical consistency between the speed of sound predicted by the excitation spectrum, and the speed of sound obtained from the hydrodynamic derivative of the equation of state. The procedure, whose only visible effect is that it avoids spurious damping of long-wavelength phonons due to anomalous dispersion, has also been described in Ref. 28.

Four sets of results suffice to summarize the message of this paper. These are both the unrenormalized and the renormalized version of the uniform limit approximation, and the same two versions for the complete HNC evaluation of the ingredients $\mathcal{F}$, $\mathcal{G}$, and $\mathcal{R}$. The results for the dynamic structure function $S(q,\omega)$ are shown in Figs. 4–7. As a guide to

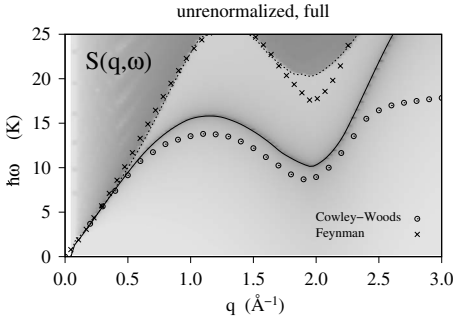

FIG. 6. Same as Fig. 4 for the HNC calculation.

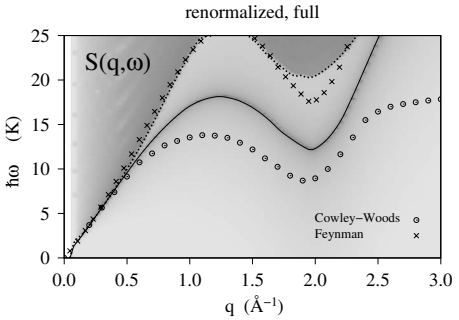

FIG. 7. Same as Fig. 5 for the HNC calculation.

where one wants to get, we also show the experimental data of Cowley and Woods[29] and the Feynman spectrum $\varepsilon(q)=\hbar^2q^2/2mS(q)$ in the figures.

These results are quite interesting and not entirely expected. The rationalization for including pair fluctuations was discussed above. In this work, we have introduced an approximation for the functions $\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$, $\mathcal{G}_{22}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)$, and $\mathcal{R}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$ that satisfies *both* properties, Eqs. (3.2) and (3.3), at the same time. Nevertheless, the combined effect of all of these improvements is quite small. In the CA, the roton minimum comes out at 12.1 K which is somewhat lower that the value of 12.9 K reported in Ref. 9. We have traced the discrepancy to a different treatment of "elementary diagram" contributions in the ground-state calculation. The "renormalization" raises that energy to 13.3 K. On the other hand, the HNC calculation of the two-body operators lowers the roton minimum to 10.2 K in the unrenormalized version whereas the renormalization raises it again to 12.2 K, i.e., to almost the same location that was predicted by the simplest, time-honored version of Chang and Campbell.[12]

One might, at this point, of course question the validity of the integral equations employed here for the calculations of the basic ingredients of the theory. These equations sum just the *minimum* sets diagrams that one must include in order to guarantee both the correct long- and the short-ranged structure of these quantities. But we already have experience with the additional quantities, triplet correlations and elementary diagrams, in ground-state calculations. The total effect is not negligible but by far not large enough to bridge the gap between the calculated and the experimental roton energy. Further evidence for the fact that our approximations are sufficient is the fact that the leading corrections to the right-hand side $\mathcal{R}(\mathbf{r}_1;\mathbf{r}_1,\mathbf{r}_3)$ are indeed negligible; see the discussion at the end of Sec. III.

Thus, the only conclusion is that the truncation of the excitation operator at the two-body level is insufficient for explaining the experimental data. The cause for this is already seen in the self-energy in the CA, Eq. (2.51): the energy denominator contains just the Feynman excitation energies. When three-body fluctuations are included at the same level, the energy denominator gets modified into[23]

$$\hbar\omega-\Sigma[|\mathbf{q}/2-\mathbf{p}|,\hbar\omega-\varepsilon(|\mathbf{q}/2+\mathbf{p}|)]-\Sigma[|\mathbf{q}/2+\mathbf{p}|,\hbar\omega-\varepsilon(|\mathbf{q}/2+\mathbf{p}|)]. \quad (4.1)$$

That means that the energies in the energy denominator get basically shifted close to the energies of the experimental phonon-roton spectrum. We have occasionally simulated this effect in previous work by scaling the energy denominator accordingly. The above result justifies this procedure; it also makes clear that the shift is indeed due to triplet and possibly higher-order fluctuations.

To summarize, we have presented in this work a complete solution of the pair equation of motion for the small-amplitude dynamics of ^{4}He. Although the result that pair excitations alone can *not* explain the experimental roton energy seems disappointing at first glance, it is actually quite encouraging: it comes with the message that the CA is, unexpectedly, quite good even far beyond the roton momentum. The diagrammatic resummations carried out above are, while numerically not challenging in the homogeneous geometry, demanding in nonuniform systems. Thus it is good news that the CA, while at first glance defeating the purpose of many-body fluctuations, is quite accurate. Moreover, one can also expect that triplet fluctuations can be dealt with at the same level of approximation which makes even the implementation of the theory for inhomogeneous systems such as films and clusters feasible.

ACKNOWLEDGMENTS

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APPENDIX A: MOMENTUM SPACE EQUATIONS

The Fourier transform of $\mathcal{F}_{22}(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)=\mathcal{F}_{22}(\mathbf{r}_{12},\mathbf{r}_{13})$ is defined as

$$\tilde{\mathcal{F}}_{22}(\mathbf{p}_1,\mathbf{p}_2)=\rho^2\int d^3r_{12}d^3r_{13}e^{i\mathbf{p}_1\cdot\mathbf{r}_{12}-i\mathbf{p}_2\cdot\mathbf{r}_{13}}\mathcal{F}_{22}(\mathbf{r}_{12},\mathbf{r}_{13}). \quad (A1)$$

With this convention, the three integral Eqs. (3.4)–(3.6) become

$$\tilde{\mathcal{F}}_{22}^{(N)}(\mathbf{p}_1,\mathbf{p}_2)=\tilde{\mathcal{F}}_{22}^{(\mathrm{CA})}(\mathbf{p}_1,\mathbf{p}_2)+\tilde{h}(\mathbf{p}_2)\tilde{\mathcal{F}}_{22}^{(X)}(\mathbf{p}_1,\mathbf{p}_2),$$

$$\tilde{\mathcal{F}}_{22}^{(X)}(\mathbf{p}_1,\mathbf{p}_2)=\int\frac{d^3p_3}{(2\pi)^3\rho}\tilde{h}_2(\mathbf{p}_1-\mathbf{p}_3)\tilde{\mathcal{F}}_{22}^{(N)}(\mathbf{p}_3,\mathbf{p}_2),$$

$$\tilde{\mathcal{F}}_{22}^{(\mathrm{CA})}(\mathbf{p}_1,\mathbf{p}_2)=(2\pi)^3\rho\delta(\mathbf{p}_1-\mathbf{p}_2)S(p_1). \quad (A2)$$

The four-point function also depends parametrically on $\mathbf{q}$,

$$\tilde{\mathcal{G}}_{22}^{(N)}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2)=\tilde{\mathcal{G}}_{22}^{(\mathrm{CA})}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2)+\tilde{s}_{\mathbf{q}}(\mathbf{p}_1)\tilde{\mathcal{G}}_{22}^{(X)}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2),$$

$$\tilde{\mathcal{G}}_{22}^{(X)}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2)=\int\frac{d^3p_3}{(2\pi)^3\rho}\tilde{h}_2(\mathbf{p}_1-\mathbf{p}_3)\tilde{\mathcal{G}}_{22}^{(N)}(\mathbf{q};\mathbf{p}_3,\mathbf{p}_2),$$

$$\tilde{\mathcal{G}}_{22}^{(\mathrm{CA})}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2)=(2\pi)^3\rho\delta(\mathbf{p}_1-\mathbf{p}_2)S(|\mathbf{q}/2-\mathbf{p}_1|)S(|\mathbf{q}/2+\mathbf{p}_1|) \quad (A3)$$

with

$$\tilde{s}_{\mathbf{q}}(\mathbf{p}) = S(|\mathbf{q}/2+\mathbf{p}|)S(|\mathbf{q}/2-\mathbf{p}|) - 1. \tag{A4}$$

The integral equation for the right-hand side is practically the same with a different driving term

$$\tilde{\mathcal{R}}^{(N)}(\mathbf{q};\mathbf{p}) = \tilde{\mathcal{R}}^{(\mathrm{CA})}(\mathbf{q};\mathbf{p}) + \tilde{s}_{\mathbf{q}}(\mathbf{p})\tilde{\mathcal{R}}^{(X)}(\mathbf{q};\mathbf{p}),$$

$$\tilde{\mathcal{R}}^{(X)}(\mathbf{q};\mathbf{p}) = \int \frac{d^3p'}{(2\pi)^3\rho}\tilde{h}_2(\mathbf{p}-\mathbf{p}')\tilde{\mathcal{R}}^{(N)}(\mathbf{q};\mathbf{p}'),$$

$$\tilde{\mathcal{R}}^{(\mathrm{CA})}(\mathbf{q};\mathbf{p}) = \tilde{h}_2(|\mathbf{q}/2-\mathbf{p}|)\tilde{h}_2(|\mathbf{q}/2+\mathbf{p}_1|) + \tilde{u}_3(|\mathbf{q}/2-\mathbf{p},\mathbf{q}/2+\mathbf{p}_1,-\mathbf{q}\,|). \tag{A5}$$

The inhomogeneity of the pair equation is in momentum space

$$\tilde{\mathcal{V}}^{(3)}(\mathbf{q},\mathbf{p}) = \frac{\hbar^2}{2m}\mathbf{q}\cdot\left[\left(\frac{\mathbf{q}}{2}+\mathbf{p}\right)\tilde{h}_2\left(\frac{\mathbf{q}}{2}+\mathbf{p}\right) + \left(\frac{\mathbf{q}}{2}-\mathbf{p}\right)\tilde{h}_2\left(\frac{\mathbf{q}}{2}-\mathbf{p}\right) + \mathbf{q}\tilde{\mathcal{R}}(\mathbf{q};\mathbf{p})\right]. \tag{A6}$$

The convolution approximation of all three quantities consists of just keeping the terms labeled with a superscript (CA).

The full kinetic-energy operator needs some more work. We start from the integral equation and expand the fluctuation in momentum space. First split off the center-of-mass motion as given in Eq. (2.49). Then the coordinate space representation of the kinetic-energy operator in Eq. (2.25) becomes

$$-\frac{\hbar^2}{2m}\left(i\frac{\mathbf{q}}{2}+\nabla_1\right)\cdot\int d^3\rho_3\mathcal{F}_{22}(\mathbf{r}_{12},\mathbf{r}_{13}) \times\left(i\frac{\mathbf{q}}{2}+\nabla_1\right)\delta v_{\mathbf{q}}(\mathbf{r}_1-\mathbf{r}_3)e^{i\mathbf{q}\cdot(\mathbf{r}_3-\mathbf{r}_2)/2} \tag{A7}$$

or, in momentum space

$$\frac{\hbar^2}{2m}\int\frac{d^3p_1}{(2\pi)^3\rho}\tilde{\mathcal{F}}_{22}(\mathbf{q}/2+\mathbf{p}_1,\mathbf{q}/2+\mathbf{p}_2) \times(\mathbf{q}/2-\mathbf{p}_1)\cdot(\mathbf{q}/2-\mathbf{p}_2)\bar{v}_{\mathbf{q}}(\mathbf{p}_2). \tag{A8}$$

The second kinetic-energy term is the same with the signs of $\mathbf{p}$ and $\mathbf{k}$ reversed. Thus, the momentum space representation of the kinetic-energy operator becomes

$$\tilde{T}_{22}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2;\omega) = \frac{\hbar^2}{2m}(\mathbf{q}/2+\mathbf{p}_1)\cdot(\mathbf{q}/2+\mathbf{p}_2)\tilde{\mathcal{F}}_{22}(\mathbf{q}/2-\mathbf{p}_1,\mathbf{q}/2-\mathbf{p}_2) + \frac{\hbar^2}{2m}(\mathbf{q}/2-\mathbf{p}_1)\cdot(\mathbf{q}/2-\mathbf{p}_2)\tilde{\mathcal{F}}_{22}(\mathbf{q}/2+\mathbf{p}_1,\mathbf{q}/2+\mathbf{p}_2). \tag{A9}$$

APPENDIX B: PARTIAL-WAVE EXPANSIONS

The momentum space equations are solved in angular momentum representation. We need, as an auxiliary quantity, the partial-wave expansion

$$\tilde{h}_2(|\mathbf{k}_1-\mathbf{k}_2|) = \sum_{\ell m}\frac{4\pi}{2\ell+1}\tilde{h}_\ell(k_1,k_2)Y_{\ell m}(\Omega_1)Y^*_{\ell m}(\Omega_2), \tag{B1}$$

where the Ω_i are the angles between $\hat{\mathbf{k}}_i$ and $\hat{\mathbf{q}}$. We also need the partial-wave expansion of $\tilde{s}_{\mathbf{q}}(\mathbf{p})$ defined in Eq. (A4),

$$\tilde{s}_{\mathbf{q}}(\mathbf{p}) = \sum_{\ell\ \mathrm{even}} s_\ell(p)P_\ell(\hat{\mathbf{q}}\cdot\hat{\mathbf{p}}). \tag{B2}$$

The partial-wave expansion of $\tilde{s}_{\mathbf{q}}(\mathbf{p})$ defined in Eq. (B2) is generated from the partial-wave expansion of $\tilde{h}_2(\mathbf{q}/2-\mathbf{p})$. From symmetry we conclude that the $\tilde{s}_\ell(q,k)$ are zero for odd ℓ. Since the external momentum $\mathbf{q}$ enters only parametrically, we omit this dependence for ease of writing.

The right-hand side $\tilde{\mathcal{V}}(^{(3)}\mathbf{q},\mathbf{p})$ of the equation of motion can, for symmetry reasons, only depend on the values of q, p, and the angle between them. It is therefore legitimate to expand

$$\tilde{\mathcal{V}}^{(3)}(\mathbf{q},\mathbf{p}) = \sum_{\ell\ \mathrm{even}} V^{(3)}_\ell(q,p)P_\ell(\hat{\mathbf{q}}\cdot\hat{\mathbf{p}}), \tag{B3}$$

where, due to the symmetry $\mathbf{q}\leftrightarrow-\mathbf{q}$, only even angular momentum components contribute. Therefore, the excitation function also contain only even angular momentum components,

$$\delta\bar{v}_{\mathbf{q}}(\mathbf{k}) = \sum_{\ell\ \mathrm{even}} P_\ell(\hat{\mathbf{q}}\cdot\hat{\mathbf{k}})\,\delta\bar{v}_\ell(q,k). \tag{B4}$$

1. Four-body term

The operator $\tilde{\mathcal{G}}_{22}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2)$ can be generated by iteration as indicated in Eq. (A3). Owing to the symmetries discussed above, we can write

$$\tilde{\mathcal{G}}_{22}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2) = \sum_{\ell_1\ell_2\ \mathrm{even}} G_{\ell_1\ell_2}(p_1,p_2)P_{\ell_1}(x_1)P_{\ell_2}(x_2) \tag{B5}$$

and likewise for $\tilde{\mathcal{G}}^{(\mathrm{CA})}_{22}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2)$, $\tilde{\mathcal{G}}^{(N)}_{22}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2)$, and $\tilde{\mathcal{G}}^{(X)}_{22}(\mathbf{q};\mathbf{p}_1,\mathbf{p}_2)$. In angular momentum decomposition, we have

$$\tilde{G}^{(X)}_{\ell_1,\ell_2}(p_1,p_2) = \frac{1}{2\ell_1+1}\int\frac{d^3p_3}{(2\pi)^3\rho}h_{\ell_1}(p_1,p_3)G^{(N)}_{\ell_1,\ell_2}(p_3,p_2),$$

$$\tilde{G}^{(N)}_{\ell_1,\ell_2}(p_1,p_2) = G^{(\mathrm{CA})}_{\ell_1,\ell_2}(p_1,p_2) + (2\ell_1+1)\sum_{\ell_3}\Sigma_{\ell_1\ell_3}(p_1) \times G^{(X)}_{\ell_3\ell_2}(p_1,p_2),$$

$$\tilde{G}^{(\mathrm{CA})}_{\ell_1,\ell_2}(p_1,p_2) = \frac{(2\pi)^3\rho}{4\pi}\delta(p_1-p_2)[(2\ell_1+1)\delta_{\ell_1,\ell_2} + (2\ell_1+1)(2\ell_2+1)\Sigma_{\ell_1,\ell_2}(p_1)], \quad \text{(B6)}$$

where

$$\Sigma_{\ell_1\ell_2}(p_1) = \sum_\ell s_\ell(p_1)\begin{pmatrix}\ell & \ell_1 & \ell_2\\ 0 & 0 & 0\end{pmatrix}^2. \quad \text{(B7)}$$

2. Right-hand side

Inserting the partial-wave expansion in Eq. (A5) gives basically the same equation for the components of

$$\tilde{\mathcal{R}}(\mathbf{q};\mathbf{p}) = \sum_{\ell \text{ even}} R_\ell(q)P_\ell(\hat{\mathbf{q}}\cdot\hat{\mathbf{p}}), \quad \text{(B8)}$$

$$\tilde{R}^{(N)}_\ell(p) = \tilde{R}^{(\mathrm{CA})}_\ell(p) + (2\ell+1)\sum_{\ell'}\Sigma_{\ell\ell'}(q/2,k)\tilde{R}^{(X)}_{\ell'}(k),$$

$$\tilde{R}^{(X)}_\ell(k) = \frac{1}{2\ell+1}\int\frac{d^3p}{(2\pi)^3\rho}\tilde{h}_\ell(k,p)\tilde{R}^{(N)}_\ell(p), \quad \text{(B9)}$$

and $\tilde{R}^{(\mathrm{CA})}_\ell(p)$ is the partial-wave expansion of the $\tilde{R}^{(\mathrm{CA})}(\mathbf{q},\mathbf{p})$ defined in Eq. (A5). From the solution of Eq. (B9) we obtain the partial-wave expansion, Eq. (B3), by adding the partial-wave expansion of the first two terms in the definition, Eq. (A6). Again, for symmetry, we conclude that only even-ℓ terms contribute.

3. Three-body term

$\tilde{\mathcal{F}}_{22}(\mathbf{q}/2-\mathbf{p}_1,\mathbf{q}/2-\mathbf{p}_2)$ is a function of the angles $\hat{\mathbf{q}}\cdot\hat{\mathbf{p}}_1$, $\hat{\mathbf{q}}\cdot\hat{\mathbf{p}}_2$, and $\hat{\mathbf{p}}_1\cdot\hat{\mathbf{p}}_2$. We can, in this term, not use the argument that only the $m=0$ components contribute to the integral equation because we can couple an $m=1$ component with the factors $(\mathbf{q}/2-\mathbf{p}_1)\cdot(\mathbf{q}/2-\mathbf{p}_2)$ in Eq. (A8) to an $m=0$ component. We must therefore expand into spherical harmonics $Y_{\ell m}(\Omega_1)$ and $Y_{\ell' m}(\Omega_2)$, where Ω_1 and Ω_2 are the angles between $\mathbf{p}_1$ and $\mathbf{q}$ or $\mathbf{p}_2$ and $\mathbf{q}$, respectively. Note that the m quantum number is the same: this comes from the fact that $\tilde{\mathcal{F}}_{22}(\mathbf{q}/2-\mathbf{p}_1,\mathbf{q}/2-\mathbf{p}_2)$ is only a function of $|\mathbf{q}/2-\mathbf{p}_1|$, $|\mathbf{q}/2-\mathbf{p}_2|$, and $|\mathbf{p}_1-\mathbf{p}_2|$. Hence,

$$\tilde{\mathcal{F}}_{22}(\mathbf{q}/2-\mathbf{p}_1,\mathbf{q}/2-\mathbf{p}_2) = \sum_{\ell_1\ell_2 m}\frac{4\pi}{\sqrt{(2\ell_1+1)(2\ell_2+1)}} \times F_{\ell_1\ell_2 m}(p_1,p_2)Y_{\ell_1 m}(\Omega_1)Y^*_{\ell_2 m}(\Omega_2). \quad \text{(B10)}$$

The partial-wave expansions for $\tilde{\mathcal{F}}^{(X)}_{22}$ and $\mathcal{F}^{(N)}_{22}$ are defined in the same way. Inserting this into the integral Eq. (A2) gives the angular momentum representation

$$\tilde{F}^{(N)}_{\ell_1\ell_2 m}(p_1,p_2) = \tilde{F}^{(\mathrm{CA})}_{\ell_1\ell_2 m}(p_1,p_2) + (2\ell_2+1) \times\sum_{\ell_3}\tilde{F}^{(X)}_{\ell_1\ell_3 m}(p_1,p_2)\Gamma_{\ell_2\ell_3 m}(p_2),$$

$$\tilde{F}^{(X)}_{\ell_1\ell_2 m}(p_1,p_2) = \frac{1}{2\ell_2+1}\int\frac{d^3p_3}{(2\pi)^3\rho}\tilde{F}^{(N)}_{\ell_1\ell_2 m}(p_1,p_3)\tilde{h}_{\ell_2}(p_2,p_3),$$

$$\tilde{F}^{(\mathrm{CA})}_{\ell_1\ell_2 m}(p_1,p_2) = \frac{(2\pi)^3\rho}{4\pi}\delta(p_1-p_2)[(2\ell_1+1)\delta_{\ell_1,\ell_2} + (2\ell_1+1)(2\ell_2+1)\Gamma_{\ell_1,\ell_2 m}(p_1)], \quad \text{(B11)}$$

with

$$\Gamma_{\ell_1\ell_2 m}(p) = (-1)^m\sum_\ell h_\ell(q/2,p)\begin{pmatrix}\ell & \ell_2 & \ell_3\\ 0 & m & -m\end{pmatrix}\begin{pmatrix}\ell & \ell_2 & \ell_3\\ 0 & 0 & 0\end{pmatrix}. \quad \text{(B12)}$$

We need to solve these equations only for $m=0$ and $m=1$. To calculate the kinetic-energy operator, we must combine the partial-wave expansion, Eq. (B10), with the factor $(\mathbf{q}/2-\mathbf{p}_1)\cdot(\mathbf{q}/2-\mathbf{p}_2)$ and recouple the angular momenta. This is straightforward and can be omitted here.

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