International Journal of Theoretical Physics, Vol. 25, No. 3, 1986

Toward a Comprehensive Theory for He II. I. A Zero-Temperature Hybrid Approach

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Received June 12, 1984

A simple hybrid approach, based on a gauge theory as well as a Hartree formalism, is presented for He II at zero temperature. Although this is intended to be merely a first step in an all-embracing theory, it already resolves quite neatly several old inconsistencies and corrects a few errors. As an illustration of its feasibility, a crude but instructive calculation is performed for the static structure factor of the system at low momentum transfers. A number of planned extensions and generalizations are outlined.

1. INTRODUCTION

That He II has been at the center of a lively area of research is an indisputable fact; that it is still a most intriguing system, both experimentally and theoretically, is evident in any recent low-temperature conference, for example, the Vienna Symposium (Neutron Inelastic Scattering, 1978) and the Low Temperature Conferences (Proceedings of LT-15, 1978; Proceedings of LT-16, 1981).

The reason for this lies in its remarkable thermohydrodynamic behavior (Putterman, 1974), in spite of its extreme atomic simplicity (Bethe & Salpeter, 1957). After all, next to hydrogen, the helium atom is the lightest and simplest. The question then arises: How can such a system with almost the simplest elementary constituents and interatomic forces display such an intricate and rich macroscopic behavior?

One glaring aspect of this behavior of He II is, of course, its superfluidity, which has hitherto eluded a satisfactory microscopic understanding. The most pertinent riddle in this connection is the threefold relation: Bose–Einstein condensation superfluidity, order parameter superfluidity, and He–He interaction superfluidity (London, 1964; Brewer, 1965; Tilley and Tilley, 1974; Chester, 1975). This theme far transcends He II itself,

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0020-7748/86/0300-0255$05.00/0

since superfluidity seems to be the norm rather than the exception in low-temperature physics. For one thing, it occurs in both Fermi as well as Bose systems; for another, it characterizes not only neutral but also charged systems. According to recent speculations and hypotheses, we may even have "supersolids" (Reatto, 1969; Chester, 1970; Leggett, 1970; Saslow, 1977) and "supergases" (Stwalley and Nosanow, 1976; Crampton et al., 1979; Silvera and Walraven, 1980), illustrating all the more emphatically the fundamental nature of this peculiar phenomenon and its pervasiveness (Mendelssohn, 1956; Ginzburg, 1978; Chela-Flores, 1978).

Another equally glaring aspect of the macroscopic behavior of He II is that it exhibits apparent features of a gas and a solid, besides those of a liquid (London, 1964; Khudeir, 1981). We recall here that its structure (Achter and Meyer, 1969; Hallock, 1972; Robkoff and Hallock, 1981; Svensson et al., 1980), represented by the pair correlation function $g(r)$ and the static structure factor $S(Q)$, conforms by and large with the familiar pattern of a simple liquid (Pryde, 1966; Egelstaff, 1967; Temperley et al., 1968; March and Tosi, 1976). Yet it is very strongly interacting (the short-range part of the interatomic potential being several orders of magnitude greater than typical liquid energies) and highly dense (in the sense that the range of the interaction is comparable with the interparticle separation) (Woo, 1976; Bishop et al., 1977). The constituent particles are therefore so closely packed as if the system were a solid. This is even more transparent in its energy spectrum (Woods and Cowley, 1970, 1971), especially in the phonon branch which is reminiscent of the well-known acoustic branch in the dispersion relation of lattice vibrations in crystals (Kittel, 1976): He II seems to behave like a solid which has lost some of its rigidity. Paradoxically enough, however, it behaves in some other respects like a gas of almost noninteracting particles. For example, its molar volume at absolute zero ($=27.6\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$) (Donnelly, 1967) is more than three times the volume calculated from the known He–He interaction (Bishop et al., 1977). This is a consequence of the relatively large zero-point motion of the helium atoms, which leads to an expanded structure in which they can move quite freely over appreciable distances (Kittel and Kroemer, 1980).

This peculiar "trichotomy" of behavior may have been the principal reason behind the diversity of microscopic models and theories professing to account for the bizarre properties of He II—ranging from the nearly independent-particle type [as in Bogoliubov's pioneering work (Bogoliubov, 1947), and the fairly successful wave-theoretic approach of Gross (Gross, 1963a; Gross, 1963b; Gross, 1966) and Pitaevskii (Pitaevskii, 1961)], to the lattice-model variety [for instance, Thouless' attempt to treat the system as a disordered quantum solid (Thouless, 1969)]. However, none can be said to embody the long-awaited microscopic theory of liquid helium; Landau's phenomenological theory (Landau, 1941, 1947) seems to have fared much better.

In fact, the hydrodynamic theory of He II has recently received a new impetus, following the development of various variational methods for deriving generalized two-fluid equations (Lhuillier et al., 1975; Geurst, 1976; Jackson, 1978, 1979), which may readily incorporate the effects of applied electric fields (Jackson, 1982) and are apparently suitable for treating a wider class of systems, such as ^{3}He–^{4}He mixtures, normal and superfluid ^{3}He, superconductors and classical fluids, including plasmas. The importance of this cannot be overemphasized, since it has been felt for some time now that a unified theory of these systems is overdue. They share with each other some striking similarities, although there exist conspicuous differences as well.

This work initiates yet another approach along the same broad lines. It is the first of a planned series of papers aiming ultimately at formulating a comprehensive theory of He II, with possible extensions to the other systems just mentioned. The main idea is to adopt a hierarchy of successive approximations as different facets of the theory are gradually learned. From this standpoint, our theory should at present be judged on the basis of its potentialities, rather than any actual achievements.

The long-term strategy is as follows. In this paper, I, we shall lay the foundations at absolute zero, borrowing in the process a few seminal ideas from quantum-field theory, and eliminating certain inconsistencies and errors in related previous work. In the second paper, II (Chela-Flores and Ghassib, 1986), we shall generalize the theory to arbitrary temperatures and establish the underlying gauge-theoretical aspects on a more solid ground. In subsequent papers, we shall work out in detail the thermohydrodynamics of He II, hoping to reconsider some long-standing problems and modify the theory to accommodate other related systems.

A partial list of these problems appears, together with a general discussion, in Section 4 of the present paper. Prior to this, the basic ingredients of the theory are set out, with special emphasis on the physical import of the key equations (Section 2), and a crude but illuminating calculation is presented for the liquid structure factor at low momentum transfer (Section 3). The relevant mathematical details are collected together in an appendix.

2. BASIC THEORY

We first wish to revisit the old Hartree model of Gross and Pitaevskii for He II (Gross, 1963a, 1963b, 1966; Pitaevskii, 1961). Apart from its aesthetic appeal as an exceedingly simple starting point, this model has long provided a most fruitful framework for exploring a wide variety of vortex phenomena and ion mobility in this system. However, its central assumption of the validity of a mean-field theory is clearly at odds with the strongly interacting nature of liquid helium. Moreover, it presupposes the presence of a substantial Bose-Einstein condensate—again in harmony with an almost-independent-boson model, rather than real He II. In this connection, we remark that, following a period of uncertainty as to the existence of a condensate in He II (Jackson, 1974; Hyland and Rowlands, 1977) recent evidence has once again tilted in favor of the condensate (Sears et al., 1982): At 1 K, 13% of the ^{4}He atoms seem to lie in the lowest-momentum state. However, the precise relation of this condensate fraction to superfluidity is still a moot point.

In this work our underlying philosophy is to use the field equations beyond their normal range of validity, thereby disregarding their Hartree origins. Besides, we circumvent the need to assume the existence of a specific condensate fraction by treating Bose-Einstein condensation and superfluidity as two distinct phenomena, the latter being viewed as an *operational* concept, defined by a set of clear-cut operations, such as the remarkable property of nonclassical rotational inertia (Yang, 1962; Kohn and Sherrington, 1970). The crucial new element introduced here is the adoption of a gauge theory (Chela-Flores, 1975; Chela-Flores, 1976; Chela-Flores, 1977), which should go a long way toward justifying our method.

Prior to developing this theme, however, it is necessary to summarize the key points of the conventional Gross-Pitaevskii picture.

2.1. The Conventional Approach

As already stated, this is a nearly-independent-particle model which ignores the short-range interatomic correlations. Strictly speaking, then, it cannot be applicable to He II. Nonetheless, the fact that it has been extensively applied to this system, with some undeniable successes (Gross, 1966), implies that there must be more than a modicum of truth in it.

This may not be all that surprising, thanks to the gaslike properties of He II (Donelly, 1967; Kittel and Kroemer, 1980). A concession to the nonideal characteristics of the system is made by introducing a purely repulsive δ-function interaction, in the manner of Bogoliubov's classical work (Bogoliubov, 1947).

Notwithstanding this interaction, most particles apparently remain in the same zero-momentum state, thereby forming a condensate. In passing, we note, with Bogoliubov himself, that the choice of a zero-momentum state as the ground, or lowest-momentum, state is a mere reflection of the specific choice of the reference frame, which is taken here as the condensate itself.

Accordingly, instead of representing the systems by the usual permanent

$$\Psi(\mathbf{x}, t) = \prod_{i=1}^{N} \psi_i(\mathbf{x}, t)$$

we can describe it quite adequately by any single-particle wave function $\psi(\mathbf{x}, t)$. This so-called condensate wave function satisfies the nonlinear Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(\mathbf{x}, t) = -\tfrac{1}{2}\nabla^2\psi(\mathbf{x}, t) + \psi(\mathbf{x}, t)\int V(\mathbf{x}-\mathbf{x}')|\psi(\mathbf{x}', t)|^2\, d\mathbf{x}' \tag{1}$$

and is normalized according to

$$\int |\psi(\mathbf{x}, t)|^2\, d\mathbf{x} = N \tag{2}$$

where N is the total number of particles. Here and throughout we use a system of units such that $\hbar = m_4$ (the mass of a ^{4}He atom) = 1, the conversion factor being $\hbar^2/m_4 = 12.1194$ K Å^2.

Much has been written about the condensate wave function (Brewer, 1966; Tilley and Tilley, 1974). In the conventional approach, it may be viewed most simply as a *coherent field* with negligible fluctuations, the condensate being macroscopically occupied. Although this picture is clearly inconsistent with our own philosophy, we shall still start with equation (1), as explained below.

The hydrodynamics follows from a Madelung transformation (Putterman, 1974; Shönberg, 1954; Wong, 1976), namely,

$$\psi(\mathbf{x}, t) = R(\mathbf{x}, t)\exp[iS(\mathbf{x}, t)] \tag{3}$$

where $R(\mathbf{x}, t)$ is a real function related to the *local* density of the system (Gross, 1966), $\rho = |R|^2$, and the phase $S(\mathbf{x}, t)$ is another real quantity intimately linked with the velocity field, as we shall see. It is worth noting that the simultaneous determination of R (or, equivalently, ρ) and S is possible, even though N and S are conjugate variables obeying an uncertainty relation for any quantum system (Tilley and Tilley, 1974; Anderson, 1966), because N is exceedingly large here. Substituting equation (3) into (1), and equating real and imaginary parts, we finally obtain the continuity equation:

$$\frac{\partial}{\partial t}R^2(\mathbf{x}, t) + \nabla\cdot[R^2(\mathbf{x}, t)\nabla S(\mathbf{x}, t)] = 0 \tag{4}$$

from the imaginary part, and the Bernoulli equation

$$-R(\mathbf{x}, t)\frac{\partial}{\partial t}S(x, t) + \frac{1}{2}\nabla^2 R(\mathbf{x}, t) = E[V]R(\mathbf{x}, t) \tag{5}$$

from the real part, $E[V]$ being a functional of the interaction:

$$E[V] \equiv \tfrac{1}{2}[\nabla S(\mathbf{x}, t)]^2 + \int V(\mathbf{x}-\mathbf{x}')R^2(\mathbf{x}', t)\,d\mathbf{x}' \qquad (6)$$

Clearly, considered as an eigenvalue problem, equation (5) with $E[V]=0$ describes the nonsuperfluid ideal Bose gas. We shall return to this problem shortly.

2.2. Present Formalism

The point of departure of this work from the conventional approach just outlined is that we propose to base our study of the II on the field equations (4)-(6), supplemented with equations (2) and (3), irrespective of their origins. In particular, we inject into the formalism various aspects of a gauge theory (Chela-Flores, 1975); ours may therefore be regarded as a hybrid approach. The claim is that *gauge invariance is a fundamental symmetry of nature* (Weinberg, 1975), from which there follows the desired ψ function describing superfluid helium. It will be recalled, in this respect, that equation (1) has invariance of the first kind (Gross, 1966). We now assume that invariance of the second kind (Utiyama, 1956) also holds and hence aim at deriving the whole theory from an action principle, in which the coupling of the gauge field to ψ is dictated by symmetry requirements. This follows closely the steps of Yang and Mills (Yang and Mills, 1954); in our case, however, we shall have the benefit of a much simpler Abelian theory—unlike the comparatively more sophisticated non-Abelian theory of, say, isospin symmetry. We shall present the full derivation and elaborate on the principles involved in paper II (Chela-Flores and Ghassib, 1986), where the temperature will also be brought into the picture.

For the time being, the gauge-theoretic approach [in the limit of a vanishing gauge field (Chela-Flores, 1975)] may be viewed as a mere variational formulation of the Hartree liquid model which invokes an appropriate Lagrangian density, subject to a gauge constraint dictated by quantum field theory. Evidently, a shrewd guess of the Lagrangian density is crucial here. Chela-Flores' choice (Chela-Flores, 1975) was directly inspired by the Gross-Pitaevskii formalism (Gross, 1963a; Pitaevskii, 1961); other choices, based on entirely different considerations, may also be possible, the corresponding field equations being obtained when the prescribed "crank is turned." Thus, we have a scheme of successive approximations in which the present choice (Chela-Flores, 1975) of Lagrangian density is only the first step.

Returning to equation (6): The first term on the right can be thought of as a kinetic energy $p^2/2$. A plausible interpretation, then, is that ∇S is the "superfluid momentum" of the system $\mathbf{p}_s$, which is also the velocity $\mathbf{v}$ in our system of units. Alternatively, equation (5) may be regarded as an eigenvalue equation; it can be reexpressed in the compact form

$$(\Box - E[V])R = 0 \tag{7}$$

with

$$\Box \equiv -\partial S/\partial t + \tfrac{1}{2}\nabla^2 \tag{8}$$

The eigenvalue problem summarized in equation (5)-(8) seems to be rich in content. In the first place, if it turns out that this problem does indeed describe He II, or at least some aspects of its behavior, as we claim, then we must infer that superfluidity is closely associated with the two terms on the right-hand side of equation (6). This is not as far fetched as it may seem: The term $(\nabla S)^2/2$ is simply $v^2/2$, as we have seen, and it should therefore be reminiscent of Landau's criterion for superfluidity (Landau, 1941, 1947); moreover, the interaction term is expected to play a crucial role in this connection, judging from all previous studies [for example, Bogoliubov's original work (Bogoliubov, 1947)].

In the second place, equation (7) is Bernoulli-like (Putterman, 1974; Lamb, 1932). It can be rewritten as

$$-\partial S/\partial t = (\nabla S)^2/2 + \pi(\mathbf{x}, t) \tag{9}$$

Dividing throughout by the volume of the system (assumed to be unity for simplicity), we can see at once that each term in this equation is essentially a pressure. In particular, the left-hand side $(-\partial S/\partial t)$ may readily be interpreted as the internal pressure of the system; henceforth we shall refer to it as the *Bernoulli pressure.* Further, $\pi(\mathbf{x}, t)$ is defined as

$$\pi(\mathbf{x}, t) \equiv -\frac{1}{2}\frac{\nabla^2 R}{R} + \int V(\mathbf{x}-\mathbf{x}')R^2(\mathbf{x}', t)\, d\mathbf{x}' \tag{10}$$

where the first term on the right is the so-called quantum pressure (Gross, 1963a; Gross, 1963b; Gross, 1966), and the second is some effective pressure arising from the effects of the binary He-He potential.

Now, on switching off the interaction V, the term $(\nabla S)^2/2$ in equation (9) cancels out exactly the quantum-pressure term in equation (10). Thus, the Bernoulli pressure in our zero-temperature formalism vanishes for the ideal Bose gas—as expected, since all the particles will then be in the zero-momentum state and will not, therefore, exert any force on the walls of the container. On the other hand, when V is switched on, the Bernoulli pressure will be some positive number. This will be relatively large for a purely repulsive (positive) potential; whereas it will be small if an attractive (negative) component is added to the potential. It seems, then, that the

Bernoulli pressure can be regarded as a crude qualitative guide to the effects of the He–He interaction on the hydrodynamics of the system. This conclusion is sufficiently interesting to merit a more careful investigation.

Other significant effects can also be deduced from equation (7), such as the well-known Josephson effects (Tilley and Tilley, 1974), which arise when two volumes of bulk He II are connected by a weak link, in complete analogy with two bulk superconductors weakly coupled together. We note, in passing, that if the gradient of both sides of equation (7) is taken, Newton's second law for the "superfluid" particles will immediately be obtained.

Finally, the potentialities of the above approach may be illustrated by using equation (7) to probe the atomic structure of He II. This constitutes the main theme of the next section.

3. A CRUDE CALCULATION FOR $S(Q)$

We examine here equation (7) in its velocity-linearized version, for a stationary fluid, with a purely repulsive δ-function $V(\mathbf{x}-\mathbf{x}')=U\delta(\mathbf{x}-\mathbf{x}')$. To simplify the mathematics further, we consider only the long-wavelength limit, corresponding to small momentum transfers Q, and adopt a spherically symmetric solution.

What do these approximations entail? The first simply implies that only low fluid velocities are permitted, so that the quadratic term in $\mathbf{v}$, $(\nabla S)^2/2$, is ignored. The second means that the velocity potential $(-\partial S/\partial t)$ can be set equal to a constant, E_v, say. The long-wavelength limit is precisely the region under present investigation. And a spherically symmetric solution indicates that the local density $\rho(\mathbf{x})=\rho(r)=R^2(r)$, where the dependence on t has now been dropped. All these are perfectly plausible approximations which should lead to a physically sound result.

However, the δ-function interaction is a somewhat different matter. Although its use is perhaps fully justified in studying phenomena whose characteristic lengths are much larger than the range of the interparticle force, such as vortices (Gross, 1963a; Gross, 1966), this can hardly be the case in the present context, involving as it does the atomic order of He II. The fine structure of the He–He potential is bound to be important, since the ^{4}He atoms can easily explore it by virtue of their large zero-point motion arising from their very light masses. Besides, the crucial role of Fröhlich's attractive electron-phonon interaction (Fröhlich, 1950) in the microscopic theory of superconductivity (Bardeen et al., 1957) is a poignant warning that the weakly attractive (Van de Waals) tail of the He–He counterpart cannot be suppressed with impunity. Of more immediate relevance to the present calculation is the fact that the attractive part primarily determines the density of the system, among other properties (Yang, 1970), so that the absence of this part is inconsistent with the use of the experimental density. This point is worth remembering in the analysis of our results. In short, then, the employment of the δ-function interaction here is dictated by mathematical convenience, rather than by physical considerations. It may be viewed as an apt starting point for an eventual systematic investigation, based on a hierarchy of more and more refined interactions (Bishop et al., 1977; Aziz et al., 1979).

With the above approximations, equation (7) reduces at once to the following equation of motion for the local density $\rho(r)$:

$$\rho U - E_v - \nabla^2(\rho^{1/2})/(2\rho^{1/2}) = 0 \tag{11}$$

or

$$2\rho^{3/2}U - 2E_v\rho^{1/2} - \frac{\partial^2}{\partial r^2}\rho^{1/2} = 0 \tag{12}$$

This can be readily solved by direct integration (Chela-Flores, 1977)—noting that (i) as $r \to \infty$, $\rho \to \rho_\infty = \text{const}$, which is nothing but the particle density of the bulk system; and (ii) for $r \leq r_0$, $\rho = 0$, r_0 being the "effective" hard-core radius. The respective experimental values are (Wilks, 1967; Mountain and Raveché, 1973) $\rho_\infty = 0.1450\ \text{g/cm}^3 = 2.18 \times 10^{-2}$ particles Å^{-3}, and $r_0 = 2.0$ Å. The solution, subject to these boundary conditions, is

$$\rho(r) = \rho_\infty \tanh^2[\Lambda(r_0 - r)] \tag{13}$$

with

$$\Lambda \equiv (\rho_\infty U)^{1/2} \tag{14}$$

so that the corresponding radial distribution function is simply

$$g(r) = \rho(r)/\rho_\infty = \tanh^2[\Lambda(r_0 - r)] \tag{15}$$

This expression is clearly a reflection of the gaslike aspects of the model adopted. However, some liquid effects can be incorporated through the parameter Λ just defined. We have attempted to do this by considering two alternative approaches. The first consists in comparing equation (15), for several values of Λr_0, with the experimental curve for $g(r)$ (Achter and Meyer, 1969). It turns out that a value of ≈ 4.0 is not unreasonable for Λr_0. Needless to say, this is *not* a parameter-fitting exercise; the experimental curve is viewed here as a mere guide. A more rigorous comparison is hardly necessary under the present circumstances.

The second approach invokes the familiar expression for a two-body pseudopotential (Huang, 1963; Pathria, 1972):

$$U\delta(r) = 4\pi a_0 \delta(r) \tag{16}$$

in our system of units, where a_0 is the relevant S-wave scattering length (Joachain, 1979). A most appropriate value for $|a_0|$ is ≈ 2.1 Å, which pertains to the so-called Sposito potential (Bishop et al., 1977; Sposito, 1970). This was constructed such that its short-range part reproduces the repuslive potential deduced from the experimental high-energy ^{4}He-^{4}He scattering data; whereas its long-range component has the correct asymptotic (dipole-dipole and dipole-quadrupole) behavior. Unlike all the other He-He potentials available in the literature, however, the Sposito potential was adjusted so as to yield the *measured* ground-state energy of liquid ^{4}He, when combined with the virial theorem, and with the *experimental* $g(r)$. It follows that the choice of its scattering length introduces some liquid effects. We can now compute the parameter Λ from equations (14) and (16):

$$\Lambda = (4\pi a_0 \rho_\infty)^{1/2} = 0.75 \text{ Å}^{-1}$$

so that $\Lambda r_0 = 1.5$, which is of the same order of magnitude as the value given by the first approach.

Having determined $g(r)$, we can obtain the corresponding liquid structure factor $S(Q)$ by simply plugging equation (15) in the definining equation (March and Tosi, 1976)

$$S(Q) = 1 + \frac{4\pi\rho}{Q} \int_0^\infty [g(r) - 1] r \sin(Q_r)\, dr \tag{17}$$

where $\mathbf{Q}$ is the scattering wave vector specifying the momentum transfer to the medium. Thus,

$$S(Q) = 1 - \frac{4\pi\rho}{Q} \int_0^\infty \operatorname{sech}^2[\Lambda(r_0 - r)] r \sin(Qr)\, dr \tag{18}$$

For small Q, it is shown in the Appendix that equation (18) reduces to

$$S(Q) = S_0 + S_2 Q^2 + O(Q^3) \tag{19}$$

with

$$S_0 \equiv 1 - 4\pi\rho_\infty r_0^3 f_1 \qquad \text{and} \qquad S_2 \equiv 4\pi\rho_\infty r_0^5 f_2 \tag{20}$$

f_1, f_2 being some numerical factors. For $\Lambda r_0 \geq 5.2$, a fairly satisfactory agreement with experiment (Hallock, 1972) is obtained; whereas for lower values of Λr_0 such an agreement is possible only if ρ_∞ is regarded as a floating parameter to be determined by fitting the theoretical with the experimental curve. Curiously enough, a rather similar conclusion is drawn in previous work (Chela-Flores, 1977) about the value $\Lambda r_0 \approx 5.2$. However, in view of some inaccuracies and errors in that work, the similarity involved here must be fortuitous. [In particular, alluding to (Chela-Flores, 1977), the integral in equation (24) should be preceded by a factor of $(\Lambda r_0)^{-1}$; the signs in equation (3) of Appendix C are all wrong; the integral $I_\alpha \equiv \int_0^\alpha x^2 \operatorname{sech}^2 x \, dx$ is evaluated inaccurately; and the value of the fluid density is underestimated by a factor of ≈ 20.] Equations (19) and (20) represent our central result. Any improvements or refinements in the present calculation should ultimately manifest themselves in an even better agreement with experiment. For the time being, the above semiquantitative success remains the best that can be achieved within our modest framework. Nevertheless, it is essentially a low-density (gas) result. Accordingly, it should also follow from an appropriate virial expansion (Keller, 1969; Larsen et al., 1965; Bruch, 1969). Crude estimates based on available experimental data for the second virial coefficient (Hirschfelder et al., 1964; Mason and Spurling, 1969) seem to support this.

4. SUMMARY AND DISCUSSION

In this work we have constructed a hybrid theory for He II based on the Gross–Pitaevskii model as well as a more recent gauge formalism. The new theory seems to be superior to either approach in that it resolves quite neatly a few old inconsistencies and difficulties in this domain without marring the essential simplicity of the picture involved.

As an illustration of the potentialities of our theory, we have computed the liquid structure factor for small momentum transfers using a set of sharply defined approximations. The result agrees with experiment to a satisfactory extent, considering the limited range of validity of these approximations. In this respect, several prospective generalizations suggest themselves.

The first concerns the interparticle potential V, whose importance can hardly be overexaggerated. As already pointed out, its fine structure is probably vital in atomic-order calculations. However, the use of realistic potentials (Bishop et al., 1977; Aziz et al., 1979; Sposito, 1970) renders the computations rather involved. Thus, while aiming eventually at employing such potentials, one may approach this problem in the short run by repeating the calculation of $S(Q)$ for other more refined models than the δ function—for instance, the so-called (pure) boundary condition model (Feshbach and Lomon, 1964). This is a nontrivial, although still fairly simple, potential which may be expressed as the sum of a suitable repulsive step function and an attractive δ function (Kim and Tubis, 1970). It is therefore a better simulation of the He–He interaction.

Other generalizations follow by relaxing the set of approximations introduced to simplify the calculations. The hope here is to extend the range of validity of $S(Q)$ beyond the small Q limit. A particularly worthy goal in this connection is to try and establish a general relation between $S(Q)$ and the excitation energy of He II over the entire spectrum of Q, in the spirit of Bijl's pioneering effort (Bijl, 1940; Mihara and Puff, 1968; Khanna and Sinha, 1977). It is interesting to see how far one could go along these lines within the extended framework of our approach (Chela-Flores and Ghassib, 1986).

Another perennial problem is the further development of the hydrodynamic theme. This is a vast field (Putterman, 1974). The idea is to exploit any analogies and correspondences with classical hydrodynamics, in the hope of presenting eventually a complete and self-consistent treatment of superfluid hydrodynamics.

These, along with other problems of long standing mentioned in the Introduction, should ultimately enhance our understanding of the profound bonds between microscopic and macroscopic quantum phenomena. It is precisely here that we still face our most serious challenge.

ACKNOWLEDGMENTS

The authors are grateful to Professor Norman H. March for valuable advice and to Professor Julián Chela-Flores for reading the manuscript. One of them (H. B. G) is also indebted to Professor Abdus Salam, the international Atomic Energy Agency, and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste, where this work was started.

APPENDIX: EVALUATION OF $S(Q)$ FOR SMALL Q

The liquid structure factor $S(Q)$ is given, according to the present model, by equation (18). With the change of variable

$$x = \Lambda(r - r_0)$$

together with the definitions

$$y \equiv Qr_0, \qquad \alpha \equiv \Lambda \quad \beta \equiv \alpha^{-1}$$

Equation (18) reduces at once to

$$Q[S(Q) - 1]/4\pi\rho_\infty r_0^2 = -\beta I$$

where I is the integral

$$I \equiv \int_{-\alpha}^{\infty} (1 + \beta x) \operatorname{sech}^2 x \sin[y(1 + \beta x)]\, dx$$

or, using the addition formula for $\sin(A+B)$,

$$I=\int_{-\alpha}^{\infty}\operatorname{sech}^2 x \sin y \cos(\beta xy)\,dx+\int_{-\alpha}^{\infty}\operatorname{sech}^2 x \sin(\beta xy)\cos y\,dx$$

$$+\beta\int_{-\alpha}^{\infty}x\operatorname{sech}^2 x\sin y\cos(\beta xy)\,dx+\beta\int_{-\alpha}^{\infty}x\operatorname{sech}^2 x\sin(\beta xy)\cos y\,dx$$

This can be simplified further by splitting each of the four integrals into two: one of the form $\int_{-\alpha}^{0} f(x)\,dx$, and another of the form $\int_{0}^{\infty} f(x)\,dx$. Altogether, then, we have eight integrals: four "finite" (i.e., with a finite upper limit) and four "infinite" (the upper limit being ∞).

Now, in the low-Q region under discussion here, we can use $\cos y\approx 1$ and $\sin y\approx y$ in all of these eight integrals. Moreover, in the finite integrals *only*, we can set $\sin(\beta xy)\approx\beta xy$ and $\cos(\beta xy)\approx 1$. It follows that, in this region,

$$I=I_{\text{finite}}+I_{\text{infinite}}$$

where, after some trivial manipulations,

$$I_{\text{finite}}=y\int_{0}^{\alpha}\operatorname{sech}^2 x\,dx-2\beta y\int_{0}^{\alpha}x\operatorname{sech}^2 x\,dx+\beta y\int_{0}^{\alpha}x^2\operatorname{sech}^2 x\,dx$$

and

$$I_{\text{infinite}}=y\int_{0}^{\infty}\operatorname{sech}^2 x\cos(\beta xy)\,dx+\int_{0}^{\infty}\operatorname{sech}^2 x\sin(\beta xy)\,dx$$

$$+\beta y\int_{0}^{\infty}x\operatorname{sech}^2 x\cos(\beta xy)\,dx+\beta\int_{0}^{\infty}x\operatorname{sech}^2 x\sin(\beta xy)\,dx$$

For I_{finite}: The first term yields by direct integration,

$$y(\tanh x)_0^{\alpha}=y\tanh\alpha$$

the second gives, on integration by parts,

$$-2\beta y(x\tanh x-\ln\cosh x)_0^{\alpha}=-2\beta y(\alpha\tanh\alpha-\ln\cosh\alpha)$$

whereas the third term is best evaluated by numerical integration, since the validity of the analytic solution obtained (Gradshteyn and Ryzik, 1965) in terms of Bernoulli numbers (Abramowitz and Stegun, 1965) is severely restricted by convergence difficulties. We have found that a simple method, such as Simpson's rule with a fairly coarse mesh [say, $0(0.1)\alpha$], is more than adequate in this connection. For reference purposes we list in Table AI the integral $I_\alpha\equiv\int_0^{\alpha}x^2\operatorname{sech}^2 x\,dx$ for several values of α.

Table AI. The Integral $I_\alpha \equiv \int_0^\alpha x^2 \operatorname{sech}^2 x \, dx$ for Several Values of α

α	I_α
1.0	0.20
4.0	0.81
5.2	0.82

On the other hand, I_{infinite} can be evaluated analytically; the individual integrals are simply the Fourier cosine and sine transforms of the functions $\operatorname{sech}^2 x$ and $x \operatorname{sech}^2 x$. The result, to $\sim O(y^3)$, is (Erdelyi, 1954)

$$I_{\text{infinite}} = y\left(1 - \frac{\pi^2}{24}\beta^2 y^2\right) + [\beta y \ln 2 - \tfrac{3}{16}\zeta(3)\beta^3 y^3]$$

$$+ \beta y[\ln 2 - \tfrac{9}{16}\zeta(3)\beta^2 y^2] + \beta\left(\frac{\pi^2}{12}\beta y - \frac{3\pi^4}{1440}\beta^3 y^3\right)$$

where $\xi(3)$ is the Riemann ζ function given by (Abramowitz and Stegun, 1965): $\zeta(3) = 1.20206$.

Finally, then, collecting all the above terms together and reexpressing the result in terms of Q, we obtain

$$S(Q) = S_0 + S_2 Q^2$$

with

$$S_0 \equiv 1 - 4\pi\rho_\infty r_0^3 f_1 \qquad \text{and} \qquad S_2 \equiv 4\pi\rho_\infty r_0^5 f_2$$

the factors f_1, f_2 being defined by the expressions

$$f_1 \equiv \beta(\tanh\alpha + 1) + \beta^2 I_\alpha + 2\beta^2 \ln 2 + \frac{\pi^2}{12}\beta^3 - 2\beta^2\ (\alpha\tanh\alpha - \ln\cosh\alpha)$$

and

$$f_2 \equiv \frac{\pi^2}{24}\beta^3 + \frac{3}{4}\zeta(3)\beta^4 + \frac{7\pi^4}{1440}\beta^5$$

Table AII. Numerical Results for S_0 and S_2 for Two Different Values of $\alpha \equiv \Lambda r_0$

α	β	f_1	f_2	S_0	S_1
4.0	0.25	0.56	1.0×10^{-2}	−0.24	0.09
5.2	0.19	0.42	4.3×10^{-3}	0.08	0.04

A summary of these results is presented in Table AII for two different values of $\alpha \equiv \Lambda r_0$.

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