Biophysics and the Microscopic Theory of Helium II

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Bose–Einstein condensation and solitonic propagation have recently been shown to be intimately related in biosystems. From our previous demonstration of the existence of solitons in a dilute Bose gas, we set out the basis for a full microscopic theory of He II. This is used to understand recent experiments, which are in apparent contradiction. New experiments are suggested.

1. INTRODUCTION

The original remark by London (1938) linking the phenomenon of superfluidity in He II with Bose–Einstein condensation (BEC) has inspired a great deal of theory and experiment.

On the other hand, the excitation spectrum was put on a solid microscopic basis by a remarkable variational calculation by Feynman and Cohen (FC) (1956), which connected the excitation spectrum with the dynamic structure factor obtained from inelastic neutron scattering, and at the same time pointed out the relevance of backflow.

In spite of the importance of the FC variational calculation, which was later improved upon by the calculation of the excitation spectrum of He II (Padmore and Chester, 1974), a few questions remain unanswered. Chief among these are:

1. What is the microscopic nature of He II? In particular, what is the nature of the roton?
2. Are there any new excitations contributing to the dispersion relation?
3. How good is the FC wave function?

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4. What is the connection between BEC and superfluidity?

The difficulty in obtaining completely satisfactory answers to the above questions lies partly in two experimental features of this fascinating quantum liquid, namely, (1) its elementary quanta carry no electric charge, unlike superconductors; and (2) it is not subject to magnetic effects, unlike both superconductors and liquid ^{3}He.

However, we believe some significant progress may be achieved by learning from the deep insights gained from the apparently unrelated phenomenon of the macroscopic occupation of a single mode in biosystems. The BEC of phonons, underlying the work of Fröhlich (1968), has now been shown to occur in a wide variety of biophysical phenomena, among which the most prominent are the rouleaux formation of erythrocytes, as well as a wide variety of frequency-dependent responses to microwave radiation. BEC in biosystems has also been shown to be relevant to the origin of Darwinian evolution (Chela-Flores, 1985).

With the hope of making some progress in this new direction, the present work is laid out as follows: In Section 2 we give some general considerations on the possible interconnections between biophysics and He II, so as to be able to discuss a Hamiltonian formulation of the latter. Then, in Section 3, we consider some experimental consequences of our Hamiltonian. Finally, we conclude in Section 4 with a brief statement on questions open to new experimental research.

2. BIOPHYSICS AND HELIUM II

2.1. Preliminaries

To the low-temperature physicist, it may come as a surprise to learn of the intimate connection between these BEC phenomena in living organisms and the presence of solitons, as in, for instance, energy propagation in α-helical proteins (Davydov, 1982). Yet, such a relationship has recently been shown to be essentially correct (Del Guidice et al., 1982; Tuszynski et al., 1984).

The above considerations raise the question as to whether, in other systems where BEC may occur, such macroscopic occupation of a single quantum mode is accompanied by solitons.

This progress in theoretical biology has led us to consider soliton propagation in a dilute Bose gas (Chela-Flores and Ghassib, 1987), a possible realization of which is liquid ^{4}He adsorbed on porous Vycor glass (Reppy, 1984).

In this work we begin by discussing the significance of our result that soliton solutions to the time-dependent self-consistent field equation exist

and are given by the following expression:

$$\eta(x, t) = \{[(1+\tilde{\Delta})/4c_1] \sinh[X_4 + c_1^{1/2}(x - vt)]$$

$$+ [(1+\tilde{\Delta})/4c_1] \cosh[X_4 + c_1^{1/2}(x - vt)]\}^{-1} \qquad (1)$$

where v denotes the velocity of propagation of the soliton, and

$$\tilde{\Delta} = 8m_4^2 g(\Lambda - mv^2)$$

$$c_1 = -2m_4(\Lambda - mv^2)$$

Here g denotes a coupling constant representing the effects of the He–He interaction potential, m_4 is the ^{4}He atomic mass, and Λ denotes the chemical potential. Further, X_4 is a function of m_4, g, Λ, and v. The velocity of propagation is found to have a lower bound given by

$$v_c = (|\Lambda|/m_4)^{1/2} = 122 \text{ m/sec} \qquad (2)$$

where in the numerical evaluation of the critical velocity we have used the value $\Lambda = -7.14$ K. It is gratifying to note that v_c is less than the velocity of longitudinal sound waves (i.e., the velocity of first sound v_1) for temperatures below the λ point and for pressures up to 40 atm. This is consistent with soliton propagation in molecular chains, where the inequality $v_c < v_1$ has also been shown to be valid (Davydov, 1982).

Of course, equation (1) pertains to one-dimensional systems (i.e., helium in a narrow channel, which is of interest in its own right). However, judging from the relevance of the bulk He II equation (Gross, 1963), the present solution should also be germane to bulk He II.

We must next answer the question: What is the relationship, if any, between this excitation and the phonons and rotons of the standard model for the dispersion relation? This is intimately related to questions 1–3 above.

Let us first consider the evidence from experiments on neutron scattering by rotons in liquid helium. It will be recalled that at some minimum wavenumber Q_0, the neutron data can be fitted with a parabola whose equation is (Dietrich et al., 1972)

$$E(Q) \equiv \hbar\omega(Q) = \Delta + \hbar(Q - Q_0)^2/2\mu$$

Here Δ is the minimum energy, Q_0 is the wavenumber at the minimum, μ is the effective mass, and p is the roton linear momentum ($= \hbar Q$). Measurements restricted to the wavevector region near the roton minimum have been performed over the entire pressure–temperature phase space of He II above 1.3 K. For a pressure of 1 atm and a temperature of $T = 1.26$ K, $\Delta_{\text{exp}} = 0.736$ meV. Raising the temperature by 0.4 K *lowers* the gap Δ to

0.711. This should be compared with the result of the FC variational calculation, which yields

$$(p_0/\hbar)_{FC} = 1.85 \text{ Å}^{-1}, \qquad \Delta_{FC} = 0.991 \text{ meV}$$

The experimental wavenumber Q_0 does not differ substantially from $(p_0/\hbar)_{FC}$, since

$$1.902 < (p_0/\hbar)_{exp} < 1.911 \text{ Å}^{-1}$$

in the temperature range $1.26 < T < 1.68$ K at SVP. Yet the value Δ_{FC} is considerably higher than Δ_{exp}. This situation does not improve with careful Monte Carlo calculations (Padmore and Chester, 1974).

We take the above arguments to signify the possible presence of further excitations, including solitons. This point is underlined by the fact that calculations at elevated densities have not shown the expected decrease of Δ with density, raising the question as to the excellence of the FC wave function.

These difficulties lead us to reconsider the biophysical phenomenon of phonon condensation and to look at little more closely into the analogy with He II already pointed out. We shall turn the conventional argument around and enquire whether, instead of borrowing ideas from the helium literature to understand biophysical systems, we can gain further insight into superfluid helium-4 by invoking the microscopic picture of biosystems.

2.2. A Microscopic Model for He II

In order to establish the relevant Hamiltonian, recall the physical explanation of the α-helix soliton: The energy to be transported along the proteins is stored as stretching quanta of the amide-I bond; such energy does not disperse rapidly, because localized bond energy generates longitudinal sound, which in turn acts as a potential well that traps the bond energy, thereby preventing its dispersion (Scott 1982).

This work on protein solitons suggests that we seek as a source of the He II solitons their zero-point energy, which, like metabolic energy in proteins (available from ATP molecules), is an essential feature of its quantum fluid nature. In other words, if the metabolic energy supply is cut off from a biosystem, the BE condensate is automatically depleted (i.e., death occurs); likewise, if the zero-point energy is switched off, He II loses some of its macroquantum features, especially as related to its permanent-liquid nature.

We are therefore induced to consider a microscopic description in which we have three interacting subsystems: (i) A BE condensate consisting of a finite fraction of quasiparticles kept in their lowest quantum mode;

(ii) a heat bath consisting of quasiparticles with linear momentum $p \neq 0$—a "depletion"; and (iii) an energy source (zero-point motion).

This system has, in a steady state, the following Hamiltonian corresponding to He II (Wu and Austin, 1978):

$$\mathcal{H} = \sum_i \omega_i a_i^\dagger a_i + \sum_i \Omega_i b_i^\dagger b_i + \sum_i \vartheta_i P_i^\dagger P_i$$
$$+ \tfrac{1}{2} \sum_{ijk} (\chi a_i^\dagger a_j b_k^\dagger + \chi^* a_j a_i^\dagger b_k)$$
$$+ \sum_{ij} (\lambda b_i a_j^\dagger + \lambda^* b_i^\dagger a_j) + \sum_{ij} (\xi P_i a_j^\dagger + \xi^* P_i^\dagger a_j) \qquad (3)$$

where $(a_i^\dagger, a_i)$, $(b_i^\dagger, b_i)$, and $(P_i^\dagger, P_i)$ are the creation and annihilation (boson) operators for, respectively, the BE condensate, the depletion, and the "energy pump" (zero-point energy). Notice, however, that the analogy (iii) should not be stretched too far, since living organisms are *open* systems, whereas He II is a closed system. Yet the zero-point quantum fluctuations and metabolism play roles beyond the interactions in the phenomena of superfluidity and life, respectively, through the ξ coupling with the condensate. However, the analogy remains exceedingly useful, as we shall see in the next section.

2.3. On the He II Condensate

The existence of the condensate may be shown by evaluating the rate of change of the number of quanta in the ith mode (Wu and Austin, 1978):

$$\dot{n}_i = (1/i\hbar)[n_i, H] \qquad (4)$$

with $n_i = a_i^\dagger a_i$, by inferring the expectation value $\langle \psi(t)|\eta_i|\psi(t)\rangle$, where the angular brackets refer to thermal averaging in the grand canonical ensemble describing the whole system, $|\psi(t)\rangle$ being the state vector of the whole system at time t.

It is interesting to compare this approach with both FC and Davydov. FC conjecture that the state vector $|\psi_{FC}\rangle$ is time-independent; after this they proceed to a variational calculation of the excitation spectrum. In the biophysics problem the state vector $|\psi_D(t)\rangle$ is t-dependent.

On the other hand, we find that BEC may be shown by perturbation theory, starting from equation (4) and requiring stationarity in the condensate, $\langle \dot{n}_i \rangle = 0$ (Wu and Austin, 1978). Then BEC occurs, since the zero-point energy E_0 is sufficiently large (in the sense that it is the quantity that makes the system quantal *par excellence*). The occurrence of BEC is also by virtue of the ξ coupling, just as in the analogous biophysical system. Our second-quantized Hamiltonian [cf. equation (3)] has been transformed to normal coordinates (Tuszynski *et al.*, 1984). These authors have found

that it suggests a model Hamiltonian in normal coordinates, from which the nonlinear wave equation of mean field theory may be inferred. This is precisely the equation we solved recently (Chela-Flores and Ghassib, 1987).

Before discussing the experimental consequences of the model, a limiting case should be stated: the Hamiltonian (3) yields the ideal behavior (BEC) by setting Ω_i, χ, and $\lambda = 0$, since no depletion would exist in that case.

3. EXPERIMENTAL CONSEQUENCES

Clear predictions arise from the microscopic model studied in the previous section. These model-dependent consequences fail within the scope of recent experiments:

1. First, since the zero-point energy E_0 is regarded here as the analogue of the metabolic energy, it follows that, as may occur in the living system, increments in E_0 should tend to enhance BEC. This remark deserves some clarification:

BEC should occur only beyond an initial threshold E_{c1} [cf. equations (3) and (4), which do not exclude the possibility that E_{c1} could be really small, $E_{c1} < E_0$]. Some analytic formulas have been developed for E_0, which are adequate to illustrate the behavior of the condensate; a simple expression interpolates between the low- (gas) and high- (liquid) density limits (London, 1954):

$$E_0 = 150d(R - 0.891d)^{-2}(R + 0.713)^{-1} \text{ cal/mole} \qquad (5)$$

where $R = (\Omega/N)^{1/3}$, N being the particle number, and $\tilde{\Omega}$ denotes the normalization volume of the system. Both R and d (which denotes the ^{4}He atom diameter) are expressed in angstroms. The value of d is 2.70 Å. Therefore, as the ^{4}He density increases, we expect E_0 to increase as well. This completes the clarification of the enhancement of BEC with the energy source (or density) increments.

However, from the present understanding of the model we cannot estimate the value of E_{c1}. Thus, in principle, experiments should tell us if, below a critical value of the He II density ρ_{c1}, E_0 will be sufficient for the liquid to overcome the onset of BEC.

It is then possible that at SVP, or with small external pressures, there will be superfluidity without BEC, but that, with a gentle increment of pressure beyond some value P_{c1}, BEC sets in. The reader is reminded that some biosystems—for example, yeast cells—require extra pumping beyond their natural metabolism by means of microwaves so as to yield the extraordinary increments in growth rates expected from the onset of BEC of phonons (Grundler and Keilman, 1983); recent experiments in He II may be interpreted to support our suggestions (Wirth et al., 1983).

2. Finally, it may be possible that if E_0 were sufficiently large, then beyond some critical value E_{c2} the condensate would begin to be depleted. This would occur by virtue of the corresponding increments in pressure beyond some critical value P_{c2}, which would entail density increments beyond ρ_{c2} according to equation (5).

4. CONCLUSIONS

New experiments are needed to clarify the problems raised in Section 3. Preliminary reports do suggest that there might be an eventual depletion of the condensate with pressure (Mook, 1983). This question is not settled yet. However, we think that there might be elements of truth in both experiments considered here (Wirth *et al.*, 1983; Mook, 1983).

To conclude, we may say that in view of these rather unexpected suggestions, it may be worth reconsidering the nature of the condensate, as already pointed out (Ghassib and Sridhar, 1984). We look forward to a fresh crop of experiments to clarify the uncertainties underlying the present approach.

ACKNOWLEDGMENTS

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