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BIOPHYSICS AND THE MICROSCOPIC THEORY OF He II *

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ABSTRACT

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 in He II, which are in apparant contradiction. New experiments are suggested by the microscopic theory.

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The original remark of Fritz London in 1938¹ 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 the remarkable variational calculation of Feynman and Cohen (FC),² 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 Monte Carlo calculation of the excitation spectrum of He II,³ a few questions remain unanswered. Chief among these are:

- (a) What is the microscopic nature of He II? In particular, what is the nature of the roton?
- (b) Are there any new excitations contributing to the dispersion relation?
- (c) How good is the FC wave function?
- (d) 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 ³He. 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 quantum mode in biosystems.⁴ The BEC of phonons, underlying Frohlich's seminal contribution,⁴ has now been shown to occur in a wide

variety of biophysical phenomena, amongst 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.⁵

To the low-temperature physicist, it may first 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.⁶ Not such a relationship has recently been shown to apply.⁷ This raises 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,⁸ a possible realization of which is liquid ⁴He adsorbed in porous Vycor glass.⁹ In this letter we discuss the significance of our result that soliton solutions to the time-dependent self-consistent field equation exist and are given by the following expression:⁸

$$\eta(x,t) = \left\{ \left[\frac{(1+\tilde{\Delta})}{4c_1} \sinh[X_4 + \sqrt{c_1} (x-vt)] \right] + \left[\frac{(1-\tilde{\Delta})}{4c_1} \cosh[X_4 + \sqrt{c_1} (x-vt)] \right] \right\}^{-1} \quad (1)$$

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

$$\tilde{\Delta} = 8 m_4^2 g (\Delta - m v^2) ; \\ c_1 = -2 m_4 (\Delta - m v^2).$$

where g denotes a coupling constant representing the effects of the He-He interaction potential, m_4 is the ⁴He atomic mass and Δ denotes the chemical potential. Further, X_4 is a function of a_4 , E , Δ and v . The velocity of propagation is found to have a lower bound given by

$$v_c = \sqrt{|\Delta|/m_4} = 122 \text{ m/s} \quad (2)$$

where in the numerical evaluation of the critical velocity we have used the value $|\Delta| = -7.14$ 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.⁶

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 (a) to (c) above.

Let us first consider the evidence retrieved from experiments on neutron scattering by rotons in liquid helium.¹⁰ It will be recalled that at some minimum wavenumber Q_0 , the neutron data can be fitted with the parabola

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

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

$$\left(\frac{p_0}{\hbar} \right)_{\text{FC}} = 1.85 \text{ \AA}^{-1}, \quad \Delta_{\text{FC}} = 0.991 \text{ meV}$$

The experimental wavenumber Q_0 does not differ substantially from $(p_0/\hbar)_{\text{FC}}$, since $1.902 \text{ \AA}^{-1} < (p_0/\hbar)_{\text{exp}} < 1.911 \text{ \AA}^{-1}$

in the temperature range $1.26 \text{ K} < T < 1.63 \text{ K}$ at GVP. Yet the value Δ_{GVP} is considerably higher than Δ_{exp} . This situation does not improve with careful Monte Carlo calculations.³ We take this 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 of the excellence of the BE wave function.

These difficulties lead us in the present letter to reconsider the biophysical phenomenon of phonon condensation, and to look a little closer 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 physics literature to understand biophysical systems, we can gain further insight into superfluid helium-4 by invoking the microscopic picture of biosystems.

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 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.¹¹ This suggests that we seek as the source of the He II solitons their zero-point energy which, like metabolic energy in proteins (denoted by 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 its macroscopic features.

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:¹²

$$\mathcal{H} = \sum_i \omega_i a_i^\dagger a_i + \sum_i \Omega_i b_i^\dagger b_i + \sum_i \theta_i P_i^\dagger P_i + \frac{1}{2} \sum_{jk} (\chi a_i^\dagger a_j b_k^\dagger + \chi^* a_j a_i^\dagger b_k) + \sum_{ij} (\lambda b_i a_j^\dagger + \lambda^* b_i^\dagger a_j) + \sum_i (\zeta P_i a_i^\dagger + \zeta^* P_i^\dagger a_i) \quad (3)$$

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 are playing roles beyond the interactions in the phenomena of superfluidity and life, respectively, through the ζ -coupling with the condensate. However, the analogy remains exceedingly useful as we shall see. The existence of the condensate may be shown by evaluating the rate of change of the number of quanta in the i th mode:¹²

$$\dot{n}_i = (1/it) [n_i, \mathcal{H}] \quad (4)$$

with $n_i = a_i^\dagger a_i$, by inferring the expectation value $\langle \psi(t) | \dot{n}_i | \psi(t) \rangle$, where the angular brackets refer to ther-

overlapping in the grand canonical ensemble describing the whole system, $|\Psi(t)\rangle$ being the state vector of the whole system (Eq. 3). It is instructive to compare this approach with the one of Bogoliubov and Davydov. They conjecture that the state vector $|\Psi_{FC}\rangle$ is t-independent. Then they proceed to a variational calculation of the excitation spectrum. On the biophysics problem, the state vector $|\Psi(t)\rangle$ is t-dependent. On the other hand, we find that BEC may be shown by perturbation theory, starting from Eq. (4) and requiring stationarity in the condensate, $\langle \dot{N}_1 \rangle = 0$. Then BEC occurs, since the zero-point energy (E_0) is sufficiently large and also by virtue of the λ -coupling, just as in the analogous biophysical system. Our second quantized hamiltonian for He II, \mathcal{H} , has been transformed to normal coordinates by Tuszynski et al. They 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 which we have solved recently, and found to be responsible for soliton behavior in He II [cf. Eq. (1)].

Before discussing the experimental consequences of the theory, its limiting cases should be stated: the hamiltonian, Eq. (3), yields the ideal behavior by setting Ω_c , χ and $\lambda = 0$, since no depletion would exist in that case. Further, notice that this hamiltonian is fundamentally different from the one corresponding to the BE gas, although in practice that ideal limiting case would result if the nonlinearity is switched off.

Clear predictions arise from the above microscopic theory of He II, which are within the scope of recent experiments:

(A) In the first place, since E_0 is regarded here as the "metabolic" energy of the quantum liquid, it follows that

as in the analogous biosystem, increments in E_0 should tend to enhance BEC. This deserves some clarification: BEC should occur only beyond an initial threshold E_{c1} [cf. Eqs. (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 . A simple expression interpolates between the low and high density limits:

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

where $R = (\bar{\Omega} / N)^{1/3}$, N being the particle number, and $\bar{\Omega}$ the (normalization) volume of the system. Both R and the parameter d , denoting the helium-4 atom diameter, are expressed in angstroms; $d = 2.70 \text{ \AA}$. Therefore, as the ^4He density increases we expect E_0 to increase as well. This completes the above-mentioned clarification of the enhancement of BEC with the energy source (or density) increments. However, from the present understanding of the theory we cannot estimate the value of E_{c1} . Thus, in principle, experiments should tell us if, beneath 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 biosystems - for example, yeast cells - require extra pumping beyond its natural metabolism by means of microwaves, so as to yield the extraordinary increments in growth rates, expected from the onset of BEC of phonons. Recent experiments in He II may be interpreted to support our prediction.

(B) In the second place, it is possible that if E_0 is sufficiently large then beyond some critical value E_{c2} the con-

condensate begins 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 Eq. (5).

New experiments are needed to clarify these questions. Preliminary reports do suggest that there might be an eventual depletion of the condensate with pressure increments.¹⁶ This question is not settled yet. However, we think there might be elements of truth in both experiments considered here.^{15,16}

To conclude we may say that in view of these rather unexpected deductions, it is worth reconsidering the nature of the condensate, as has already been suggested in previous work.¹⁷ We look forward to a fresh crop of experiments to clarify the uncertainties underlying the present theory.

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