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MICROSCOPIC DERIVATION OF THE LOW-LYING EXCITATION SPECTRUM OF AN INTERACTING BOSE SYSTEM*

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Summary. - The low-lying excitation spectrum of an interacting Bose system is derived directly from the N-body microscopic Hamiltonian expressed in terms of local densities and currents as quantum-mechanical coordinates.

Long ago Feynman (1) derived an important relationship between the elementary excitation spectrum of the low-lying states of a Bose system and its correlation function for the density fluctuations: $\omega(\underset{\sim}{k}) = k^2/2mS(\underset{\sim}{k})$. This result was obtained by Feynman as a consequence of a special choice of the wave function and a subsequent variational calculation. Although the range of validity of the Feynman wave function is not quite clear (2), this result is supported by the saturated sum-rule argument of Pines (3), and the hydrodynamic derivation of Pitaevskii (4). Among these derivations, that of Pitaevskii is simplest and most concise.

Recently, however, doubt has been cast on the validity of the local velocity operator upon which the Landau theory of quantum hydrodynamics is based (5). Thus the consistency of the Pitaevskii theory is likewise open to question, since its dynamical variables are those of the Landau theory. The purpose of this note is to present an N-body microscopic derivation of the Feynman result, which is in the spirit of the Pitaevskii theory, but not subject to the objectionable use of a quantum-mechanical velocity field.

As a motivational preliminary to a theory of hadron dynamics, Dashen and Sharp (6) have demonstrated that the nonrelativistic quantum mechanics of a system of N spinless identical particles may be described completely and exactly by a theory in which the dynamical variables are the local density and currents. Unlike previous theories which are based on a density description of the system (7), no dynamical variable canonically conjugate to the density operator is introduced (8).

The expression for the Hamiltonian of a system of N identical spinless bosons (of unit mass) interacting through a local two-body potential is, in the language of second quantization, given by

$$(1) \qquad H = \frac{1}{2}\int d^3x \, \nabla\psi^+(\underset{\sim}{x}) \, \nabla\psi(\underset{\sim}{x}) \; ,$$

$$+ \frac{1}{2}\iint d^3x \, d^3y \, \psi^+(\underset{\sim}{x}) \, \psi^+(\underset{\sim}{y}) \, V(|\underset{\sim}{x}-\underset{\sim}{y}|) \, \psi(\underset{\sim}{x}) \, \psi(\underset{\sim}{y}) \; .$$

The field operators $\psi^+(\underset{\sim}{x})$ and $\psi(\underset{\sim}{x})$ satisfy the usual canonical commutation relations:

$$(2) \qquad [\psi^+(\underset{\sim}{x}), \psi^+(\underset{\sim}{y})] = [\psi(\underset{\sim}{x}), \psi(\underset{\sim}{y})] = 0 \; ,$$

$$[\psi(\underset{\sim}{x}), \; \psi^+(\underset{\sim}{y})] = \delta(\underset{\sim}{x} - \underset{\sim}{y}) \; .$$

In the second-quantized formalism, the local density and current operators are given by

$$(3) \qquad \rho(\underset{\sim}{x}) = \psi^+(\underset{\sim}{x}) \, \psi(\underset{\sim}{x}) \; ,$$

$$\underset{\sim}{J}(\underset{\sim}{x}) = \frac{1}{2i}[\psi^+(\underset{\sim}{x}) \, \nabla\psi(\underset{\sim}{x}) - \nabla\psi^+(\underset{\sim}{x}) \, \psi(\underset{\sim}{x})] \; .$$

Although $\rho(\underset{\sim}{x})$ and $\underset{\sim}{J}(\underset{\sim}{x})$ are not canonically conjugate variables, together they provide a set of quantum-mechanical coordinates that is complete (9) and they satisfy the following algebra:

$$(4) \qquad [\rho(\underset{\sim}{x}),\ \rho(\underset{\sim}{y})] = 0 \ ,$$

$$[\rho(\underset{\sim}{x}),\ J_i(\underset{\sim}{y})] = -i \frac{\partial}{\partial x_i} [\delta(\underset{\sim}{x} - \underset{\sim}{y})\ \rho(\underset{\sim}{x})] \ ,$$

$$[J_i(\underset{\sim}{x}),\ J_j(\underset{\sim}{y})] = -i \frac{\partial}{\partial x_j} [\delta(\underset{\sim}{x} - \underset{\sim}{y})\ J_i(\underset{\sim}{x})] + i \frac{\partial}{\partial y_i} [\delta(\underset{\sim}{x} - \underset{\sim}{y})\ J_j(\underset{\sim}{x})] \ .$$

Using the crucial identities

$$\underset{\sim}{\nabla} \rho(\underset{\sim}{x}) + 2i\ \underset{\sim}{J}(\underset{\sim}{x}) = 2\psi^+(\underset{\sim}{x})\ \underset{\sim}{\nabla} \psi(\underset{\sim}{x}) \ ,$$

$$\underset{\sim}{\nabla} \rho(\underset{\sim}{x}) - 2i\ \underset{\sim}{J}(\underset{\sim}{x}) = 2\underset{\sim}{\nabla} \psi^+(\underset{\sim}{x})\ \psi(\underset{\sim}{x}) \ ,$$

one may write the Hamiltonian (1) in terms of the observable quantities $\rho(\underset{\sim}{x})$ and $\underset{\sim}{J}(\underset{\sim}{x})$ in the form

$$(5) \qquad H = \frac{1}{8} \int d^3x\ [\underset{\sim}{\nabla} \rho(\underset{\sim}{x}) - 2i\ \underset{\sim}{J}(\underset{\sim}{x})] \frac{1}{\rho(\underset{\sim}{x})} [\underset{\sim}{\nabla} \rho(\underset{\sim}{x}) + 2i\ \underset{\sim}{J}(\underset{\sim}{x})] + \frac{1}{2} \iint d^3x\ d^3y\ \rho(\underset{\sim}{x})\ V(|\underset{\sim}{x}-\underset{\sim}{y}|)\ \rho(\underset{\sim}{y}) \ .$$

The variables $\rho(\underset{\sim}{x})$ and $\underset{\sim}{J}(\underset{\sim}{x})$ are natural collective variables for a description of oscillatory processes in systems consisting of large numbers of interacting particles (10). In order to study the oscillation spectrum, we set $\rho(\underset{\sim}{x}) = \langle\rho\rangle + \hat{\rho}(\underset{\sim}{x})$, where $\langle\rho\rangle$ is the equilibrium or ground state average of $\rho(\underset{\sim}{x})$ (which is a constant for translationally invariant systems). With this substitution in (5), we expand to second order in $\hat{\rho}(\underset{\sim}{x})$. One obtains

$$(6)\qquad H = \frac{1}{8\langle\rho\rangle}\int d^3x[(\underset{\sim}{\nabla}\hat{\rho}(\underset{\sim}{x}))^2 + 4(\underset{\sim}{J}(\underset{\sim}{x}))^2] + \frac{1}{2}\iint d^3x\, d^3y\, (\langle\rho\rangle + \hat{\rho}(\underset{\sim}{x}))\, V(|\underset{\sim}{x}-\underset{\sim}{y}|)\, (\langle\rho\rangle + \hat{\rho}(\underset{\sim}{y})) .$$

To eliminate $\underset{\sim}{J}(\underset{\sim}{x})$, we use the equation of continuity, $\dot{\rho}(\underset{\sim}{x}) = -\underset{\sim}{\nabla}\,\underset{\sim}{J}(\underset{\sim}{x})$. We then expand the density fluctuation $\hat{\rho}(\underset{\sim}{x})$ into Fourier components:

$$\rho(\underset{\sim}{x}) = \sum_{\underset{\sim}{k}\neq 0} \hat{\rho}(\underset{\sim}{k})\, e^{i\underset{\sim}{k}\underset{\sim}{x}} ,$$

where the $k = 0$ term is omitted due to particle conservation. Thus the Hamiltonian becomes, to second order in $\rho(\underset{\sim}{k})$,

$$(7)\qquad H = \frac{1}{2}\langle\rho\rangle^2 \iint d^3x\, d^3y\, V(|\underset{\sim}{x}-\underset{\sim}{y}|) + \frac{(2\pi)^3}{2}\sum_{\underset{\sim}{k}\neq 0}\left\{[\frac{k^2}{4\langle\rho\rangle} + V(\underset{\sim}{k})]\, |\hat{\rho}(\underset{\sim}{k})|^2 + \frac{1}{k^2\langle\rho\rangle}\, |\dot{\hat{\rho}}(\underset{\sim}{k})|^2\right\} .$$

This is immediately recognized as the Hamiltonian for a system of independent harmonic oscillators with frequencies

$$(8)\qquad \omega(\underset{\sim}{k})^2 = k^2\langle\rho\rangle\left(\frac{k^2}{4\langle\rho\rangle} + V(\underset{\sim}{k})\right) .$$

Because the single particle kinetic energy is given by $T(\underset{\sim}{k}) = k^2/2$, one can write eq. (8) as

$$(9) \qquad \omega(\underset{\sim}{k}) = [T^2(\underset{\sim}{k}) + 2\langle\rho\rangle V(\underset{\sim}{k})\, T(\underset{\sim}{k})]^{\frac{1}{2}} .$$

Thus we obtain the Bogoliubov spectrum of elementary excitations as the frequency of the oscillators. The energy of each oscillator is related to its frequency by

$$E(\underset{\sim}{k}) = \omega(\underset{\sim}{k})\,(n_{\underset{\sim}{k}} + \tfrac{1}{2}) \qquad (n_{\underset{\sim}{k}} = 0,1,2,\cdots) .$$

The ground state energy of the Bose liquid is

$$E_o = \frac{1}{2}\langle\rho\rangle^2 \iint d^3x\, d^3y\, V(|\underset{\sim}{x}-\underset{\sim}{y}|) + \sum_{\underset{\sim}{k}} \frac{1}{2}\,\omega(\underset{\sim}{k}) .$$

Since the mean value of the potential energy of an oscillator in a given state is half the mean value of the total energy of the oscillator in that state, we may write

$$\frac{1}{4}\,\omega(\underset{\sim}{k}) = \frac{(2\pi)^3}{2}\left(\frac{k^2}{4\langle\rho\rangle} + V(\underset{\sim}{k})\right)\langle|\hat{\rho}(\underset{\sim}{k})|^2\rangle ,$$

where the bracket denotes a ground state average. With the help of eq. (8), we immediately obtain

$$(10) \qquad \omega(\underset{\sim}{k}) = \frac{k^2}{2S(\underset{\sim}{k})} ,$$

where

$$S(\underset{\sim}{k}) = (2\pi)^3 \frac{\langle|\hat{\rho}(\underset{\sim}{k})|^2\rangle}{\langle\rho\rangle}$$

is the Fourier component of the density correlation function. Equation (10) is exactly Feynman's result.

Thus, we have shown that the small oscillation approximation to the Dashen-Sharp Hamiltonian (5) yields the Bogoliubov spectrum independently of any special assumptions about Bose condensation, and it further provides an alternative microscopic derivation of the Pitaevskii theory. It is interesting that the phonon spectrum, which we obtain in the limit of small k values, is independent of the presence of the Bose-condensed particles. This implies a sound velocity for these quanta which is the same above and below the λ-point. This property of the spectrum is in concert with the recent neutron scattering experiments of Woods (11) on liquid ^4He. For quanta having $k < 0.38$ Å, Woods observes that the sound velocity is essentially independent of temperature through the λ-point.

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FOOTNOTES AND REFERENCES

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