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ABSTRACT.

The quantum mechanics of a system of identical interacting particles must lead to the classical hydrodynamic equations of motion at high temperatures, because of the correspondence principle. On the other hand, the behaviour of helium II shows that this is not always the case at low temperatures. In this paper it is shown that in certain cases the quantum description requires an extra parameter, which is the potential of a new velocity field superimposed on the classical motion. Expressed in semi-classical terms, the condition for the existence of this new parameter is that the probability, in the equilibrium state, of a particle having a very large de Broglie wavelength (that is, a negligible momentum) is finite. This condition is satisfied in one model of a superfluid system, a condensed Bose-Einstein gas, but not in a crystal. A tentative theoretical interpretation of two basic equations of the empirical two-fluid theory of helium II is given, in which this new parameter determines the velocity of the superfluid.

§ 1. INTRODUCTION.

BORN AND GREEN (1947, 1948) described a method of studying transport processes in a system of identical interacting particles obeying quantum mechanics by using the analogy with the corresponding classical system. Gurov (1948, 1950) carried out a similar calculation. In both cases the conclusion was that the equations of hydrodynamics and heat transfer were identical in form with the classical equations. These treatments assumed that the three quantities describing a "normal" state of the system (Born and Green 1947, Chapman and Cowling 1939) were the same as for a classical system: the density, velocity and temperature fields. In other words, if at one instant the system is in a state described by given fields of these three parameters, its state at a later time is sufficiently described by the new fields of the parameters resulting from the thermohydrodynamical equations of motion. From the correspondence principle it is clear that the three parameters of classical mechanics are sufficient in quantum mechanics at high temperatures, but, as we shall see, this is not always true at low temperatures.

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§ 2. PROPERTIES OF THE REDUCED DENSITY MATRICES.

Suppose the system consists of N identical particles of mass m interacting by central forces whose potential is U , and let the Schrödinger representative of the density matrix of the corresponding Gibbs ensemble (Dirac 1947) be

$$D(\mathbf{q}_1, \dots, \mathbf{q}_N; \mathbf{q}'_1, \dots, \mathbf{q}'_N),$$

where $\mathbf{q}_1, \dots, \mathbf{q}_N$ are the position vectors of the N particles, and D is Hermitian. The reduced density matrices, which are also Hermitian, are defined by

$$R_k(\mathbf{q}_1, \dots, \mathbf{q}_k; \mathbf{q}'_1, \dots, \mathbf{q}'_k) = [N! / (N-k)!] \times \int \dots \int D(\mathbf{q}_1 \dots \mathbf{q}_N; \mathbf{q}'_1 \dots \mathbf{q}'_k, \mathbf{q}_{k+1} \dots \mathbf{q}_N) d\mathbf{q}_{k+1} \dots d\mathbf{q}_N \dots \quad (1)$$

The equation of motion for D is

$$i\hbar \partial D / \partial t = HD - DH, \dots \dots \dots \quad (2)$$

where H is the Hamiltonian operator of the system. After setting $\mathbf{q}_2 = \mathbf{q}'_2, \dots, \mathbf{q}_N = \mathbf{q}'_N$, this may be integrated over $\mathbf{q}_2, \dots, \mathbf{q}_N$, giving

$$i\hbar \partial R_1(\mathbf{q}_1; \mathbf{q}'_1) / \partial t = -(\hbar^2 / 2m)(\nabla_1^2 - \nabla_1'^2)R_1(\mathbf{q}_1; \mathbf{q}'_1) + \int [U(\mathbf{q}_1 - \mathbf{q}_2) - U(\mathbf{q}'_1 - \mathbf{q}_2)]R_2(\mathbf{q}_1, \mathbf{q}_2; \mathbf{q}'_1, \mathbf{q}_2) d\mathbf{q}_2, \dots \dots \quad (3)$$

where $\nabla_j = \partial / \partial \mathbf{q}_j$, etc.

By using Wigner's result (Wigner 1932, Moyal 1949) that a density matrix $R_1(\mathbf{q}_1; \mathbf{q}'_1)$ corresponds to a classical probability density $F(\mathbf{x}, \mathbf{p})$ for the position \mathbf{x} and momentum \mathbf{p} of one particle such that

$$R_1(\mathbf{q}_1; \mathbf{q}'_1) \sim \int d\mathbf{p} F(\frac{1}{2}[\mathbf{q}_1 + \mathbf{q}'_1], \mathbf{p}) \exp [i\mathbf{p} \cdot (\mathbf{q}_1 - \mathbf{q}'_1) / \hbar], \dots \dots \quad (4)$$

combined with the classical result

$$F(\mathbf{x}, \mathbf{p}) \propto \exp [-\mathbf{p}^2 / 2mkT], \dots \dots \dots \quad (5)$$

or alternatively by approximately solving the Bloch equation $\partial D / \partial (kT)^{-1} = -HD$ (Husimi 1940), we obtain a high temperature approximation

$$R_1(\mathbf{q}_1; \mathbf{q}'_1) \propto \exp [-(\mathbf{q}_1 - \mathbf{q}'_1)^2 mkT / 2\hbar^2], \dots \dots \dots \quad (6)$$

for equilibrium at the temperature T . Therefore

$$\lim_{|\mathbf{q}_1 - \mathbf{q}'_1| \rightarrow \infty} R_1(\mathbf{q}_1; \mathbf{q}'_1) = 0. \dots \dots \dots \quad (7)$$

At low temperatures (7) may not be satisfied for every type of system. To see the physical significance of the failure of (7) let us assume for the moment that $R_1(\mathbf{q}_1; \mathbf{q}'_1)$ depends only on $|\mathbf{q}_1 - \mathbf{q}'_1|$ and approaches a constant value L when $|\mathbf{q}_1 - \mathbf{q}'_1| \rightarrow \infty$. Then the Fourier inverse of (4) yields a divergent integral which may be interpreted as

$$F(\mathbf{x}, \mathbf{p}) = f(\mathbf{p}) + L\delta(\mathbf{p}), \dots \dots \dots \quad (8)$$

where $f(\mathbf{p})$ is a regular function. That is to say, the probability of one particle having zero momentum is the finite fraction $L/R_1(\mathbf{x}; \mathbf{x})$. Since (8) is in fact an expression for the mean occupation numbers of single-particle levels, L must vanish (and (7) therefore be satisfied) in a Fermi-Dirac system, where the exclusion principle limits the occupation numbers.

§ 3. ASYMPTOTIC BEHAVIOUR OF THE REDUCED DENSITY MATRIX FOR ONE PARTICLE.

In the general case when (7) does not hold we shall consider the behaviour of $R_i(\mathbf{q}_i; \mathbf{q}'_i)$ for values of $|\mathbf{q}_i - \mathbf{q}'_i|$ large compared with both $\hbar(mkT)^{-1/2}$ and the range of U . The integral in (3) may be written, using the Hermitian property of R_2 ,

$$\int U(\mathbf{r})[R_2(\mathbf{q}_i, \mathbf{q}_i + \mathbf{r}; \mathbf{q}'_i, \mathbf{q}_i + \mathbf{r}) - R_2^*(\mathbf{q}'_i, \mathbf{q}'_i + \mathbf{r}; \mathbf{q}_i, \mathbf{q}_i + \mathbf{r})] d\mathbf{r}. \quad (9)$$

Suppose that the asymptotic form of $R_2(\mathbf{q}_i, \mathbf{q}_i + \mathbf{r}; \mathbf{q}'_i, \mathbf{q}_i + \mathbf{r})$ for large $|\mathbf{q}_i - \mathbf{q}'_i|$ is

$$R_2(\mathbf{q}_i, \mathbf{q}_i + \mathbf{r}; \mathbf{q}'_i, \mathbf{q}_i + \mathbf{r}) \sim A(\mathbf{q}_i, \mathbf{r})R_1(\mathbf{q}_i; \mathbf{q}'_i), \quad (10)$$

just as the neighbour distribution function of a liquid obeys

$$R_2(\mathbf{q}_1, \mathbf{q}_2; \mathbf{q}_1, \mathbf{q}_2) \sim R_1(\mathbf{q}_1; \mathbf{q}_1)R_1(\mathbf{q}_2; \mathbf{q}_2) \quad (11)$$

for large $|\mathbf{q}_1 - \mathbf{q}_2|$. For large $|\mathbf{q}_i - \mathbf{q}'_i|$ (3) becomes

$$i\hbar \partial R_1(\mathbf{q}_i; \mathbf{q}'_i) / \partial t \sim -(\hbar^2/2m)(\nabla_i^2 - \nabla_i'^2)R_1(\mathbf{q}_i; \mathbf{q}'_i) + [X(\mathbf{q}_i) - X^*(\mathbf{q}'_i)]R_1(\mathbf{q}_i; \mathbf{q}'_i), \quad (12)$$

where $X(\mathbf{q}) = \int A(\mathbf{q}, \mathbf{r})U(\mathbf{r}) d\mathbf{r} = V(\mathbf{q}) + iW(\mathbf{q}). \quad (13)$

Since the variables in (12) are separable the general solution is a linear combination of expressions of the form

$$\Psi(\mathbf{q}_i)\Psi^*(\mathbf{q}'_i), \quad (14)$$

where $i\hbar \partial \Psi / \partial t = -(\hbar^2/2m)\nabla^2 \Psi + X\Psi. \quad (15)$

At equilibrium $D = e^{-\beta H}$, and since the Schrödinger representative of H is real, those of D and the R 's are also real. The state of the liquid is uniform, and, therefore, for large enough $|\mathbf{q}_i - \mathbf{q}'_i|$ it may be assumed that

$$R_1(\mathbf{q}_i; \mathbf{q}'_i) \sim \text{const.}$$

This is of the form (14) with $\Psi = \text{const.}$ If the density matrix of a non-equilibrium state is sufficiently similar to $e^{-\beta H}$ the required solution of (12) will still be a single expression of the form (14):

$$R_1(\mathbf{q}_i; \mathbf{q}'_i) \sim \Psi(\mathbf{q}_i)\Psi^*(\mathbf{q}'_i). \quad (16)$$

The example of a condensed Bose gas may clarify the argument of this section. Equation (16) is true, with Ψ the wave-function of the single-particle state into which condensation has taken place. Husimi's formula (1940)

$$R_2(\mathbf{q}_1, \mathbf{q}_2; \mathbf{q}'_1, \mathbf{q}'_2) = R_1(\mathbf{q}_1; \mathbf{q}'_1)R_1(\mathbf{q}_2; \mathbf{q}'_2) + R_1(\mathbf{q}_1; \mathbf{q}'_2)R_1(\mathbf{q}_2; \mathbf{q}'_1)$$

is not valid for a condensed Bose gas; for example, at absolute zero, when all the particles are in the ground state,

$$R_1(\mathbf{q}_1; \mathbf{q}'_1) = \Psi(\mathbf{q}_1)\Psi^*(\mathbf{q}'_1),$$

$$R_2(\mathbf{q}_1, \mathbf{q}_2; \mathbf{q}'_1, \mathbf{q}'_2) = \Psi(\mathbf{q}_1)\Psi(\mathbf{q}_2)\Psi^*(\mathbf{q}'_1)\Psi^*(\mathbf{q}'_2).$$

The correct formula is

$$R_2(\mathbf{q}_1, \mathbf{q}_2; \mathbf{q}'_1, \mathbf{q}'_2) = R_1(\mathbf{q}_1; \mathbf{q}'_1)R_1(\mathbf{q}_2; \mathbf{q}'_2) + R_1(\mathbf{q}_1; \mathbf{q}'_2)R_1(\mathbf{q}_2; \mathbf{q}'_1) - \Psi(\mathbf{q}_1)\Psi(\mathbf{q}_2)\Psi^*(\mathbf{q}'_1)\Psi^*(\mathbf{q}'_2) \quad (17)$$

(compare London 1943). Assuming that this formula holds for non-equilibrium states, (10) and (11) may be verified, with

$$A(\mathbf{q}, \mathbf{r}) = R_I(\mathbf{q} + \mathbf{r}; \mathbf{q} + \mathbf{r}) + R(\mathbf{q}; \mathbf{q} + \mathbf{r})\Psi(\mathbf{q} + \mathbf{r})/\Psi(\mathbf{q}) - \Psi(\mathbf{q} + \mathbf{r})\Psi^*(\mathbf{q} + \mathbf{r}).$$

Madelung's transformation (1927) brings equations (15) and (16) into a form similar to the hydrodynamic equations of motion with velocity potential ϕ , density $|\Psi|^2$, external forces of potential V and a source distribution of strength $2|\Psi|^2W/\hbar$:

$$R_I(\mathbf{q}_I; \mathbf{q}'_I) \sim Q_\infty(\mathbf{q}_I; \mathbf{q}'_I) \exp \{im[\phi(\mathbf{q}_I) - \phi(\mathbf{q}'_I)]/\hbar\}, \quad \dots \quad (18)$$

where

$$\left. \begin{aligned} Q_\infty(\mathbf{q}_I; \mathbf{q}'_I) &= |\Psi(\mathbf{q}_I)| |\Psi(\mathbf{q}'_I)|, \\ \partial |\Psi|^2 / \partial t + \nabla \cdot (|\Psi|^2 \nabla \phi) &= 2|\Psi|^2 W / \hbar, \\ \partial \phi / \partial t + \frac{1}{2}(\nabla \phi)^2 + V/m &= \hbar^2 \nabla^2 |\Psi| / 2m^2 |\Psi| \simeq 0. \end{aligned} \right\} \dots \quad (19)$$

At equilibrium Q_∞ depends only on the density and temperature, so that even for non-equilibrium states it is a function of the parameters of the classical description. On the other hand, the velocity $\nabla\phi$ corresponds to no quantity in the classical description; it differs from the classical velocity in its laws of change and in being irrotational.

§ 4. THE TWO-FLUID MODEL OF HELIUM II.

The two-fluid model may be interpreted tentatively as follows: Assume that real functions $Q_n(\mathbf{q}_I; \mathbf{q}'_I)$ and $Q_s(\mathbf{q}_I; \mathbf{q}'_I)$ can be chosen, with $Q_n \rightarrow 0$ as $|\mathbf{q}_I - \mathbf{q}'_I| \rightarrow \infty$, such that if at one instant

$$\begin{aligned} R_I(\mathbf{q}_I; \mathbf{q}'_I) &= Q_n(\mathbf{q}_I; \mathbf{q}'_I) \exp \{im(\mathbf{q}_I - \mathbf{q}'_I) \cdot \mathbf{u}(\frac{1}{2}[\mathbf{q}_I + \mathbf{q}'_I])/\hbar\} \\ &+ Q_s(\mathbf{q}_I; \mathbf{q}'_I) \exp \{im[\phi(\mathbf{q}_I) - \phi(\mathbf{q}'_I)]/\hbar\} \\ &+ O(\nabla \mathbf{u}) + O(\nabla \nabla \phi). \end{aligned} \quad \dots \quad (20)$$

(where the velocities \mathbf{u} and $\nabla\phi$ do not alter appreciably in a distance $\hbar(mkT)^{-1/2}$), then at later instants it is of the same form, with new real functions Q_n, Q_s, \mathbf{u} , and ϕ . If $Q_s = 0$ this would describe a system with classical velocity field \mathbf{u} (Gurov 1948). The density is

$$\begin{aligned} \rho(\mathbf{x}) &= mR(\mathbf{x}; \mathbf{x}) = mQ_n(\mathbf{x}; \mathbf{x}) + mQ_s(\mathbf{x}; \mathbf{x}) \\ &= \rho_n(\mathbf{x}) + \rho_s(\mathbf{x}), \end{aligned} \quad \dots \quad (21)$$

and the current density (Born and Green 1948)

$$\begin{aligned} \mathbf{J}(\mathbf{x}) &= -(i\hbar/2)(\nabla_I - \nabla'_I)R_I(\mathbf{q}_I; \mathbf{q}'_I) \quad [\mathbf{q}_I = \mathbf{q}'_I = \mathbf{x}] \\ &= \rho_n(\mathbf{x})\mathbf{u}(\mathbf{x}) + \rho_s(\mathbf{x})\nabla\phi(\mathbf{x}). \end{aligned} \quad \dots \quad (22)$$

These two equations are the basis of the two-fluid theory (Landau 1941, Tisza 1947); in Landau's version the superfluid velocity is irrotational.

§ 5. EXAMPLES.

Two examples will illustrate the argument. In a crystal the single-molecule wave-functions are confined to small regions, so that (7) is true and classical ideas should explain its mechanical properties. In a condensed

Bose-Einstein gas with negligible repulsive forces and periodic boundary conditions (Bogoliubov 1947)

$$\left. \begin{aligned} R_l(\mathbf{q}_l; \mathbf{q}'_l) &= B^{-1} \sum_l n_l \exp i\mathbf{l} \cdot (\mathbf{q}_l - \mathbf{q}'_l), \\ Q_\infty(\mathbf{q}_l; \mathbf{q}'_l) &= n_0/B \neq 0, \end{aligned} \right\} \dots \dots (23)$$

where B is the volume of the container and n_l is the mean occupation number of the single-particle state whose wave-number is \mathbf{l} , given by

$$\left. \begin{aligned} n_l &= [\exp(\mathbf{l}^2 \hbar^2 / 2mkT) - 1]^{-1}, \quad [\mathbf{l} \neq 0], \\ \sum_l n_l &= N. \end{aligned} \right\} \dots \dots (24)$$

Bogoliubov claimed that such a system shows superfluidity.

We conclude that (7) is the condition for the classical equations of heat transfer and hydrodynamics to apply, and that when (7) is not satisfied a new quantity enters the equations. This quantity is the potential of a new velocity field superimposed on the classical motion.

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