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SUM RULES AND THEIR APPLICATION IN THE THEORY OF SUPERFLUID HELIUM*

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The first part of this paper is devoted to investigating the static response functions of superfluid helium in the hydrodynamic region which results in obtaining a new sum rule. Sum rules are then specialized to zero temperature and exploited to determine matrix elements of the particle creation and annihilation operators between the ground state and the one quasiparticle state in the long wavelength limit. We examine the particle distribution function and besides calculating the leading term, we are able to give a lower limit to the next one in the expansion for small wave numbers.

1. Introduction

We consider liquid helium below its lambda point, where it is characterized by the condensation of a finite fraction of particles into a particular single-particle state. The connection between the microscopic theory based upon the presence of the condensation and the phenomenological two-fluid hydrodynamical equations was first studied by BOGOLIUBOV [1] and by HOHENBERG and MARTIN [2]. In particular, in this way various sum rules in the hydrodynamical region have been obtained. In the first part of the present paper a new sum rule is derived by investigating the disturbance in the condensate and the particle density due to an external potential and particle sources.

Then, we are concerned with liquid helium at zero temperature with a homogeneous condensate. We limit ourselves to the long wavelength behaviour of the system and wish to explore the consequences of the sum rules. PINES [3] has proved that the one quasiparticle states exhaust the f-sum rule and the compressibility sum rule in the long wavelength limit and he has obtained the density fluctuation spectrum and the dynamic form factor in this limit. We extend his method to other sum rules and in this way we are able to calculate the matrix elements of particle creation and annihilation operators between the ground state and the one quasi-particle state in the long wavelength limit, without using perturbation theory and avoiding assumptions about the behaviour of self-energies. With the aid of these matrix elements we

* Dedicated to Prof. P. GOMBÁS on his 60th birthday.

can examine the particle distribution function in the long wavelength limit. The leading term obtained agrees with the result of the detailed microscopic calculation by GAVORET and NOZIÈRES [4] and has also been derived by applying quantum hydrodynamics [5]. Furthermore, we are able to give a lower limit for the next term in the expansion. Finally, we discuss the sum rules and the results in the BOGOLIUBOV approximation.

2. Sum rules

We consider liquid helium at a temperature T below the lambda temperature T_λ, where it is characterized by the condensation of a finite fraction of particles into a particular single-particle state. The condensate wave function is the average value of the particle field operator

$$\langle \psi(r,t) \rangle = \sqrt{n_0(r,t)}\, e^{i\varphi(r,t)}, \tag{1}$$

which is to be regarded as a quasi average [6] being nonzero by virtue of the broken symmetry.

We are interested in the linear response of the system disturbed slightly from equilibrium due to an external potential U and external sources η and η^* coupled to the particle field. Thus, we have a modified Hamiltonian

$$H + \delta H,$$

where

$$\delta H = \int U(r)\, n(r)\, d^3 r + \int \left(\eta(r)\, \psi^+(r) + \eta^*(r)\, \psi(r) \right) d^3 r$$

with

$$n(r) = \psi^+(r)\, \psi(r).$$

By taking

$$U(r) = U_k\, e^{ikr} + U_{-k}\, e^{-ikr}$$

with $U_k = U^*_{-k}$ and

$$\eta(r) = \eta_k\, e^{ikr} + \eta_{-k}\, e^{-ikr}$$

and by substituting

$$\psi(r) = \sum_k a_k\, e^{ikr}$$

we get

$$\delta H = U_k\, n_k + U_{-k}\, n_{-k} + \eta_k\, a_k^+ + \eta_{-k}\, a^+_{-k} + \eta_k^*\, a_k + \eta^*_{-k}\, a_{-k}. \tag{2}$$

By applying the usual procedure, one can write

$$\delta n_0^{1/2}(r) = \delta Re \langle \psi(r) \rangle = \delta n_0^{1/2}(k) e^{ikr} + \delta n_0^{1/2}(-k)\, e^{-ikr}, \tag{3}$$

where

$$\delta n_0^{1/2}(k) = \frac{1}{2}\left[\chi^s_{aa}(k, -k) + \chi^s_{a^+a}(-k, -k)\right]\eta^*_{-k} + \\ + \frac{1}{2}\left[\chi^s_{aa^+}(k, k) + \chi^s_{a^+a^+}(-k, k)\right]\eta_k + \\ + \frac{1}{2}\left[\chi^s_{an}(k, -k) + \chi^s_{a^+n}(-k, -k)\right]U_{-k} \tag{4}$$

and

$$\delta\langle n(r)\rangle = \delta n(k)\, e^{ikr} + \delta n(-k)\, e^{-ikr}, \tag{5}$$

where

$$\delta n(k) = \chi^s_{na}(k, -k)\,\eta^*_{-k} + \chi^s_{na^+}(k, k)\,\eta_k + \chi^s_{nn}(k, -k)\,U_{-k}. \tag{6}$$

Here $\chi^S_{AB}(k, k')$ denotes the static response function given by

$$\chi^s_{AB}(k, k') = \chi^s_{BA}(k', k) = P\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{\tau_{AB}(k, k', \omega)}{\omega}, \tag{7}$$

where τ_{AB} is defined by

$$\langle[A_k(t), B_{k'}(t')]\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\tau_{AB}(k, k'; \omega)\, e^{-i\omega(t-t')}. \tag{8}$$

According to the well-known compressibility sum rule [7]

$$\lim_{k\to 0}\chi^s_{nn}(k, k) = -\frac{n}{mc^2}. \tag{9}$$

Here c is the isothermal sound velocity $c^2 = m^{-1}(\partial P/\partial n)$, where P denotes the pressure.

Using invariance under time reversal and space inversion and Equs. (3)—(9) we find the following sum rules

$$\lim_{k\to 0}\chi^s_{an}(k, -k) = -\frac{n^{1/2}}{mc^2}\left(\frac{n}{n_0}\right)^{1/2}\left(\frac{\partial n_0}{\partial n}\right)_\eta \tag{10}$$

and

$$\lim_{k\to 0}\left[\chi^s_{a^+a}(k, k) + \chi^s_{aa}(k, -k)\right] = -\frac{1}{2\,mc^2}\,\frac{n}{n_0}\left(\frac{\partial n_0}{\partial n}\right)_\eta\left(\frac{\partial n_0}{\partial n}\right)_U, \tag{11}$$

where the derivatives are taken at constant temperature. The sum rule (10) is implicitly present in KRASNIKOV's paper [8] devoted to the generalization of BOGOLIUBOV's work to the non-ideal fluid. On the other hand, by using the two-fluid hydrodynamical equations the expression obtained by KRASNIKOV for $\chi^s_{a+a} + \chi^s_{aa}$ contains as unknown parameter the real part of the coefficient of the source terms in the hydrodynamical equations.

Finally let us quote the following sum rule, derived by BOGOLIUBOV [1] and HOHENBERG and MARTIN [2]

$$\lim_{k\to 0} [\chi^s_{aa^+}(k, k) - \chi^s_{aa}(k, -k)] = -\frac{2 n_0}{n_s} \frac{m}{k^2}, \tag{12}$$

where n_s is the superfluid density. The next term on the right hand side of Equ. (12) is a k independent one which could only be determined from microscopic theory or from knowing the parameters of a generalized two-fluid hydrodynamics taking into account derivatives of third order.

In the next Section we consider superfluid helium at zero temperature where the sum rules (9), (10) read

$$\lim_{k\to 0} \sum_\alpha \frac{|\langle \alpha | n_k^+ | 0 \rangle|^2}{\omega_{\alpha 0}} = \frac{n}{2 mc^2}, \tag{13}$$

$$\lim_{k\to 0} \sum_\alpha \frac{\langle 0 | a_{-k} | \alpha \rangle \langle \alpha | n_k | 0 \rangle + \langle 0 | n_k | \alpha \rangle \langle \alpha | a_{-k} | 0 \rangle}{\omega_{\alpha 0}} = \frac{n^{1/2}}{2 mc^2} \left(\frac{n}{n_0}\right)^{1/2} \left(\frac{\partial n_0}{\partial n}\right)_\eta, \tag{14}$$

where $\omega_{\alpha 0} = E_\alpha - E_0$ is the excitation energy. Furthermore from the sum of Equs. (11) and (12) we get

$$\lim_{k\to 0} \sum_\alpha \frac{|\langle 0 | a_k | \alpha \rangle|^2 + |\langle \alpha | a_k | 0 \rangle|^2}{\omega_{\alpha 0}} = \frac{n_0}{n} \frac{m}{k^2} + \frac{1}{2mc^2} \left(\frac{\partial n_0}{\partial n}\right)_\eta \left(\frac{\partial n_0}{\partial n}\right)_U + A, \tag{15}$$

where $-A$ denotes the constant term on the right hand side of Equ. (12).

3. Application of the sum rules

Our purpose in this section is to calculate the matrix elements of particle creation and annihilation operators in the long wavelength limit by means of the sum rules (13) (14), (15). For this we need the matrix elements of the density fluctuation, which were determined by PINES [3]. First let us summarize his results. From translational invariance it follows that

$$\lim_{k\to 0} \langle \alpha | \mathbf{J}_k | 0 \rangle \sim k^a, \qquad a > 0, \tag{16}$$

where $\mathbf{J}_k$ is the current density fluctuation, which is related to the density fluctuation by particle conservation:

$$\omega_{\alpha 0} \langle \alpha | n_k^+ | 0 \rangle = \mathbf{k} \, \mathbf{J}_k \tag{17}$$

Another essential point is that for a multi-particle state $|\alpha\rangle$ the excitation energy $\omega_{\alpha 0}$ tends to a finite value $\bar{\omega}$ in the long wavelength limit. Then, one finds for such a state from Equs. (16) and (17) that

$$\lim_{k \to 0} \langle \alpha | n_k^+ | 0 \rangle \sim \frac{k^{1+a}}{\bar{\omega}}, \qquad a > 0 . \tag{18}$$

It follows that the single quasiparticle state exhausts both the f sum rule [7]

$$\sum_\alpha \omega_{\alpha 0} |\langle \alpha | n_k^+ | 0 \rangle|^2 = \frac{nk^2}{2m} \tag{19}$$

and the compressibility sum rule (13) in the long wavelength limit, whence

$$\lim_{k \to 0} \omega_k = ck , \tag{20}$$

$$\lim_{k \to 0} \langle -k | n_k | 0 \rangle = \lim_{k \to 0} \langle 0 | n_k | k \rangle = \left(\frac{nk}{2\, mc} \right)^{1/2} . \tag{21}$$

Here $|k\rangle$ and ω_k denote the single quasiparticle state of momentum $\mathbf{k}$ and its energy, respectively. Equs. (18), (20) and (21) which are the results obtained by PINES [3] make possible the calculation of the matrix elements $\langle 0 | a_k | k \rangle$ and $\langle -k | a_k | 0 \rangle$ from the sum rules (14), (15) and from the relationship

$$\sum_\alpha \left(\langle 0 | a_k | \alpha \rangle \langle \alpha | n_{-k} | 0 \rangle - \langle 0 | n_{-k} | \alpha \rangle \langle \alpha | a_k | 0 \rangle \right) = n_0^{1/2}, \tag{22}$$

which is a direct consequence of the commutation relation

$$a_k \, n_{-k} - n_{-k} \, a_k = a_0 \, .$$

One can easily see by inspection of the sum rule (15) that the matrix elements $\langle 0 | a_k | \alpha \rangle$ and $\langle \alpha | a_k | 0 \rangle$ cannot be more singular than k^{-1} in the long wavelength limit. Then, using Equ. (18) it follows that the multi-particle configurations do not contribute to the sum rules (14) and (22) in the long wavelength limit and we obtain the equations

$$\langle 0|a_k|k\rangle \langle k|n_{-k}|0\rangle - \langle 0|n_{-k}|-k\rangle \langle -k|a_k|0\rangle = n_0^{1/2} + O(k^b) \tag{23}$$

$$\langle 0|a_k|k\rangle \langle k|n_{-k}|0\rangle + \langle 0|n_{-k}|-k\rangle \langle -k|a_k|0\rangle = $$
$$= n^{1/2}\left(\frac{n}{n_0}\right)^{1/2}\left(\frac{\partial n_0}{\partial n}\right)_\eta \frac{k}{2\,mc} + O(k^{1+b}), \tag{24}$$

where $b \geqq a$ (this condition will be sharpened in the following).* By using Equs. (20) and (21) we find for the leading term in the small k limit

$$\langle 0|a_k|k\rangle = -\langle -k|a_k|0\rangle = \left(\frac{n_0}{2n}\,\frac{mc}{k}\right)^{1/2}. \tag{25}$$

We note that to obtain this result it has been necessary only that the right hand side of Equ. (15) is not more singular than k^{-2}. By substituting Equs. (20) and (25) into the sum rule (15) it turns out that the one phonon state alone is responsible for the k^{-2} singular term. As a consequence the matrix elements $\langle 0|a_k|\alpha\rangle$ and $\langle\alpha|a_k|0\rangle$ for a multi-particle configuration can only be less singular than k^{-1}, which involves $b > a$.

Let us consider now the particle distribution function

$$N_k \equiv \langle 0|a_k^+ a_k|0\rangle = |\langle -k|a_k|0\rangle|^2 + \sum_\alpha{}' |\langle\alpha|a_k|0\rangle|^2, \tag{26}$$

where the primed summation symbol means that the summation is extended over the multi-particle configurations. According to our above results, the leading term of N_k in the small k limit is as follows

$$N_k = \frac{n_0}{n}\,\frac{mc}{2}\,\frac{1}{k}. \tag{27}$$

This agrees with the result by GAVORET and NOZIÈRES [4] obtained by analyzing the structure of the perturbation expansion and has also been derived in [5] by means of an application of quantum hydrodynamics. The derivation presented here in our opinion uses the weakest assumptions.

To obtain further results we have to take $a \geq 1$, the lower limit of which corresponds to assuming that $\langle\alpha|\mathbf{J}_k|0\rangle$ for a multi-particle configuration has

* From now on a is always considered to refer to multi-particle configurations.

a power series expansion in **k** [3]. In that case $b > 1$. Furthermore from the f sum rule (19) and Equ. (18) we find*

$$(\langle 0|n_k|k\rangle)^2 = \frac{1}{\omega_k}\left(\frac{nk^2}{2m} + O(k^4)\right) \tag{28}$$

and thus Equs. (23) and (24) give

$$(\langle -k|a_k|0\rangle)^2 + (\langle 0|a_k|k\rangle)^2 = \omega_k\left(\frac{n_0}{n}\frac{1}{k^2} + O(k^0)\right).$$

After substituting this into Equ. (15) we arrive at the conclusion that $\langle 0|a_k|\alpha\rangle$ and $\langle \alpha|a_k|0\rangle$ cannot be singular in the small k limit for multi-particle configurations and consequently $b \geqq 2$.

Let us assume the phonon dispersion law in the form

$$\omega_k = ck(1 + O(k^d)), \qquad d > 0.$$

Then according to Equ. (28) we have a term in $\langle 0|n_k|k\rangle$ proportional to $k^{d+1/2}$ and the solution of Equs. (23) and (24) can be written in the following form

$$\langle -k|a_k|0\rangle = -\left(\frac{n_0}{n}\frac{mc}{2}\right)^{1/2}\frac{1}{k^{1/2}} + \frac{1}{2}\left(\frac{n}{n_0}\frac{1}{2\,mc}\right)^{1/2}\left(\frac{\partial n_0}{\partial n}\right)_\eta k^{1/2} + O(k^{b-1/2}) + O(k^{d-1/2}) \tag{29}$$

and

$$\langle 0|a_k|k\rangle = \left(\frac{n_0}{n}\frac{mc}{2}\right)^{1/2}\frac{1}{k^{1/2}} + \frac{1}{2}\left(\frac{n}{n_0}\frac{1}{2\,mc}\right)^{1/2}\left(\frac{\partial n_0}{\partial n}\right)_\eta k^{1/2} + O(k^{b-1/2}) + O(k^{d-1/2}). \tag{30}$$

We recall that $b \geqq 2$. The last terms do not give contribution to Equs. (29) and (30) to the order $k^{1/2}$ if $d > 1$. (This is fulfilled by the usual expression for the phonon dispersion law, which assumes that ω_k^2 has a power series expansion in k^2 giving $d = 2$.) Then Equs. (26) and (29), together with the result that the contribution of the multi-particle configurations to N_k is not singular, give in the small k limit

$$N_k = \frac{n_0}{n}\frac{mc}{2}\frac{1}{k} + M \tag{31}$$

with

$$M \geqq -\frac{1}{2}\left(\frac{\partial n_0}{\partial n}\right)_\eta. \tag{32}$$

* We neglect the effects connected with the damping of the phonons, which being proportional to $\mathbf{k}^5$ at zero temperature (see for a review [2]) might not influence the long wavelength properties of the system to the order we are going to calculate them.

For liquid helium presumably $(\partial n_0/\partial n) < 0$, while in the BOGOLIUBOV approximation for the dilute Bose gas (see below) we have $(\partial n_0/\partial n) \approx 1$.

Finally let us examine the sum rule [9], [10]

$$\sum_{\alpha} \omega_{\alpha 0} \left(\langle 0|a_k|\alpha\rangle \langle \alpha|n_k|0\rangle + \langle 0|n_k|\alpha\rangle \langle \alpha|a_k|0\rangle \right) = \frac{n_0^{1/2} k^2}{2m} \tag{33}$$

which is a counterpart of the f sum rule coming from the continuity equation and the presence of the condensate. By inserting the results (21), (29) and (30) we can see that this sum rule is not exhausted by the one phonon mode in the long wavelength limit unless (n_0/n) is equal to $(\partial n_0/\partial n)$.

We conclude this Section with some remarks concerning the BOGOLIUBOV approximation [11]. The ground state $|0\rangle$ is the vacuum state of quasiparticles, i.e.

$$\alpha_k|0\rangle = 0 .$$

The quasiparticle operator α_k is given by the Bogoliubov canonical transformation:

$$\alpha_k = u_k a_k - v_k a_{-k}^+ ,$$

where

$$\left.\begin{matrix} u_k^2 \\ v_k^2 \end{matrix}\right\} = \frac{1}{2} \left[\pm 1 + \left(1 + \frac{m^2 c^4}{E_k^2} \right)^{1/2} \right], \tag{34}$$

$$u_k v_k = - \frac{mc^2}{2 E_k} .$$

Here E_k is the quasiparticle energy given by

$$E_k = \sqrt{c^2 k^2 + \left(\frac{k^2}{2m} \right)^2} , \tag{35}$$

where the sound velocity c is related to the interparticle potential V, taken to be k — independent in the small k region we are interested in, by

$$c^2 = \frac{n_0 V}{m} . \tag{36}$$

One can easily calculate the matrix elements between the ground state and the one quasiparticle state:

$$\langle 0|n_k|k\rangle = n_0^{1/2} (u_k + v_k) , \tag{37}$$

$$\langle 0|a_{-k}^+|k\rangle = v_k , \tag{38}$$

$$\langle 0|a_k|k\rangle = u_k , \tag{39}$$

where we have used as an abbreviation

$$|k\rangle = \alpha_k^+ |0\rangle \,.$$

Furthermore, one can easily check that (38) and (39) are the only non zero matrix elements of particle creation and annihilation operators. By substituting the expressions (34)—(39) into Equs. (22) and (33) we can see that they become identities.

In the long wavelength limit we get from Equs. (34), (35) that

$$\left.\begin{matrix} u_k \\ v_k \end{matrix}\right\} = \pm \frac{1}{\sqrt{2}} \left(\frac{mc}{k}\right)^{1/2} + \frac{1}{\sqrt{8}} \left(\frac{k}{mc}\right)^{1/2} + \dots \,.$$

It is well known that to the extent that the Bogoliubov approximation is valid, one can take $n_0 \approx n$, and c as given by Equ. (36) agrees with the macroscopic relationship for the sound velocity: $c^2 = (\partial P/\partial \varrho)$. Thus, one can easily tee that the sum rules (14) and (15) are satisfied and $A = 0$ in this approximasion. Furthermore N_k is given by Equ. (31) with $M = -1/2$ in the small k limit.

REFERENCES

1. N. N. Bogoliubov, On the Problem of Hydrodynamics of a Superfluid, Dubna preprint, 1963.
2. P. C. Hohenberg and P. C. Martin, Annals of Physics, **34**, 291, 1965.
3. D. Pines, in 1962 Cargese Lectures in Theoretical Physics, W. A. Benjamin Inc., New York, 1963; See furthermore: D. Pines, in Many-Body Theory, Syokabo, Tokyo and Benjamin, New York, 1966.
4. J. Gavoret and P. Nozières, Annals of Physics, **28**, 349, 1964.
5. R. A. Ferrell, N. Menyhárd, H. Schmidt, F. Schwabl and P. Szépfalusy, Annals of Physics, 565, 1968.
6. N. N. Bogoliubov, Quasi-averages in the Problems of Statistical Mechanics, Dubna Preprint, 1961.
7. See e.g.: D. Pines and P. Nozières, The Theory of Quantum Liquids I, W. A. Benjamin, Inc., New York, 1966.
8. V. A. Krasnikov, DAN, USSR, **174**, 1037, 1967.
9. F. de Pasquale, G. Jona-Lasinio and E. Tabet, Annals of Physics, **33**, 81, 1965.
10. H. Wagner, Z. Physik, **195**, 273, 1966.
11. N. N. Bogoliubov, J. Phys. USSR, **9**, 23, 1947. See furthermore: D. Pines, The Many-Body Problem, W. A. Benjamin, Inc., New York, 1962.

ПРАВИЛА СУММ И ИХ ПРИМЕНЕНИЕ В ТЕОРИИ СВЕРХТЕКУЧЕГО ГЕЛИЯ

П. СЕПФАЛУШИ

Резюме

Первая часть данной работы посвящена исследованию функций статической реакции сверхтекучего гелия в гидродинамической области, которое результирует в выходе новое правило сумм. Правила сумм затем специализированы к нулевой температуре и использованы при определении матричных элементов операторов рождения и уничтожения частиц между основным и одним квазичастичным состоянием в пределе большой длины волны. Проводилось исследование функции распределения частиц и кроме вычисления начального члена, удалось определить низшую границу следующего члена в выражении для маленьких волновых чисел.