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Interaction potential of a ^{3}He atom in a superfluid ^{4}He background

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The deformation of the superfluid ^{4}He ground state caused by the presence of a ^{3}He atom is described in terms of a polaron model. The parameters of the model are derived from the experimentally known spectrum of the ^{4}He elementary excitations and the static structure factor of ^{4}He. The resulting effective mass of the ^{3}He atom is calculated with the Feynman path-integral technique, and compares well with the experimental ^{3}He effective mass, on the condition that a microscopic ^{3}He-^{4}He interatomic potential is used that is consistent with the static ^{4}He structure factor. The main result of this paper is that the interatomic interaction potential, as, e.g., realized in the hypernetted-chain approach, leads to an accurate description of the deformation cloud around the ^{3}He atom.

Microscopic theories for ^{3}He-^{4}He mixtures provide an effective potential between a ^{3}He atom and the Bose liquid. This effective potential can be used in a more phenomenological approach, to make predictions for the mixture which are not easily attainable within the microscopic theory from which the effective potential is derived. The quality of the effective potential of course strongly depends on the degree of sophistication of the microscopic description of the superfluid ^{4}He.

The Bogoliubov pairing theory[1] is one of the first microscopic approximations that relates the static structure factor of superfluid ^{4}He to the matrix elements of the interatomic potential.

The pairing theory implies the Feynman-Bijl relation between the energy of the elementary excitations and the static structure factor in superfluid ^{4}He, and neglects the backflow.[2] As a consequence, it cannot simultaneously provide accurate quantitative results for the frequencies of the elementary excitations and for the static structure factor. The question then arises: should the matrix elements of the effective interatomic potential be derived from the elementary excitation energies or from the static structure factor or from some combination of both?

In the framework of the hypernetted-chain (HNC) approach, Owen[3] proposed an interatomic interaction potential in a ^{3}He-^{4}He mixture which is superior to the interatomic potential in the pairing theory in several respects. First, it stems from a theory that—at least in the long wavelength limit—reproduces both the static structure factor and the excitation frequencies for the pure ^{4}He superfluid.[4] Second, it allows us to predict the Landau parameters for the Fermi liquid formed by the ^{3}He atoms. Third, the interaction potential contains the masses and the structure factors of the components of the mixture as input parameters, and it can thus be constructed from the best available theoretical or experimental data.

Unfortunately, the evaluation of the effective mass of ^{3}He turns out to be very difficult in the HNC approach,[5] merely because higher-order correlations between the bosons have to be introduced in the wave function. As we will show below, a polaronlike theory overcomes this difficulty. The main purpose of this paper is to construct a suitable polaron model describing a ^{3}He atom in superfluid ^{4}He and then to illustrate its use by calculating the effective mass of the ^{3}He atom in the superfluid.

The operator form of the Hamiltonian contains three parts. The first part is the kinetic energy operator of the bare ^{3}He atom. The second part describes the boson field characterized by the frequencies of the elementary excitations of superfluid ^{4}He and their number operators. The third term represents the interaction of the ^{3}He atom with the excitations of the superfluid. This term is linear in the boson lowering and raising operators for an excitation with a well-defined wave vector, and contains the Fourier transform of the ^{3}He particle density together with the matrix element for the interaction between the bosons and ^{3}He.

Our aim is to describe the deformation of the superfluid ^{4}He ground state caused by the presence of a ^{3}He atom in terms of a completely defined polaron model, which opens new possibilities for calculating the static and dynamic properties of ^{3}He in superfluid ^{4}He using all the powerful techniques and tools available from polaron theory.[6]

The idea of a "polaron" type of description for ^{3}He in superfluid ^{4}He is based on the phenomenological theories of Bardeen, Baym, and Pines[7] and of Emery,[8] with different choices for the frequencies of the bosons and the interaction matrix elements, with calculations of the effective mass mostly on the basis of perturbation theory.

Specific heat experiments as well as second-sound measurements[9] indicate that the experimental effective mass of ^{3}He equals $2.3m_3$. It is clear that second-order perturbation theory is not a reliable procedure to calculate this effective mass: one can hardly trust a perturbation calculation to second order which predicts a doubling of the mass.

In order to proceed beyond second-order perturbation theory we generalize in this paper Feynman's variational approach for the polaron problem, and allow for wave-vector-dependent boson frequencies in the model (instead of the dispersionless LO-phonon frequency in the Feynman treatment of the polaron). We then calculate the effective mass of ^{3}He in superfluid ^{4}He with the Feynman trial action. As will be shown below, very good agreement with the experimental effective ^{3}He mass of $2.3m_3$ is obtained if one uses the effective interatomic ^{3}He-^{4}He potential from the HNC approach, which leads to a calculated ^{3}He mass of $2.312m_3$.

Our construction of the polaron model for a ^{3}He atom in the Bose liquid proceeds as follows. The energy operator for the excitations of the superfluid with energy $\hbar\omega(q)$ and with creation and annihilation operators $a_{\mathbf{q}}^{\dagger}$ and $a_{\mathbf{q}}$ is considered to be diagonal in the number operator, and it is assumed that the excitations are well defined. The kinetic energy operator for a ^{3}He atom is given by $p^2/2m_3$ where m_3 is the bare ^{3}He mass. We consider a very dilute mixture, in which the interaction with the other ^{3}He atoms can be neglected. The density fluctuations $\rho(\mathbf{q})$ of the superfluid are given by

$$\rho(\mathbf{q}) = \sqrt{N_4 S(q)}(a_{\mathbf{q}}^{\dagger} + a_{\mathbf{q}}). \tag{1}$$

The interaction potential $U(q)\rho(\mathbf{q})$ seen by the ^{3}He atom then leads to the well-known form $V(q)a_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}$ + H.c. for the interaction term in the Fröhlich Hamiltonian, with the interaction matrix element $V(q)$ given by

$$V(q) = U(q)\sqrt{N_4 S(q)}, \tag{2}$$

where $U(q)$ is the interatomic interaction potential between the ^{3}He atom and the ^{4}He atoms.

In the framework of the Bogoliubov pairing theory, the relation between the interatomic potential and the structure factor of the superfluid is given by[1]

$$U_{\text{pairing}}(q) = \frac{\hbar^2 q^2}{4m_4 N_4 S(q)^2}\left[1 - S(q)^2\right]. \tag{3}$$

But for the consistency reasons discussed above we propose in this paper to take this interatomic potential from the HNC approach:[3]

$$U_{\text{HNC}}(q) = -\frac{\hbar^2 q^2}{4m_4 N_4 S(q)^2}\left[S(q) - 1\right]^2 \times \left[1 + \left(1 + \frac{m_4}{m_3}\right)S(q)\right]. \tag{4}$$

We consider here the limit of a sufficiently small ^{3}He concentration, such that $S_{3,4}(q) \approx S_{4,4}(q) \approx S(q)$: the structure factors $S_{3,4}(q)$ and $S_{4,4}(q)$ only differ in the long wavelength limit,[7] where $S_{4,4}(q)$ tends to zero whereas $S_{3,4}(q)$ tends to a constant α for $q \to 0$. As argued by Owen,[3] the constant α gives the fractional difference between the volumes occupied by the ^{4}He atoms and the ^{3}He atoms, and consequently tends to zero in the limit of an extremely dilute mixture.

Figure 1 shows the absolute values of the matrix elements $V(q)\sqrt{V}$ (where V is the volume of the mixture) as obtained from the Bogoliubov pairing theory and from the HNC approximation, using for $S(q)$ the experimental structure factor.[10] The noise in the matrix elements stems from the experimental uncertainties in the structure factor (no smoothing was performed). It should be noted that there are major quantitative differences between both approximations: the matrix elements from the HNC scheme are smaller and faster decaying as a function of wave vector than those from the pairing theory. This indicates that the effective interaction potential is of shorter range in the pairing theory than in the HNC scheme.

Apart from both approximations considered here, we mention that, in some cases, even much less justified contact potentials[11] are used to describe the interaction of a ^{3}He atom (or an ion) with superfluid ^{4}He, with their strength *fitted* to obtain the effective mass in the framework of a perturbation scheme. In view of the structure in the effective potential, revealed by both microscopic theories discussed above, a contact potential is clearly an oversimplification of this interaction, and hardly allows to make any quantitative prediction of the ^{3}He properties in superfluid ^{4}He.

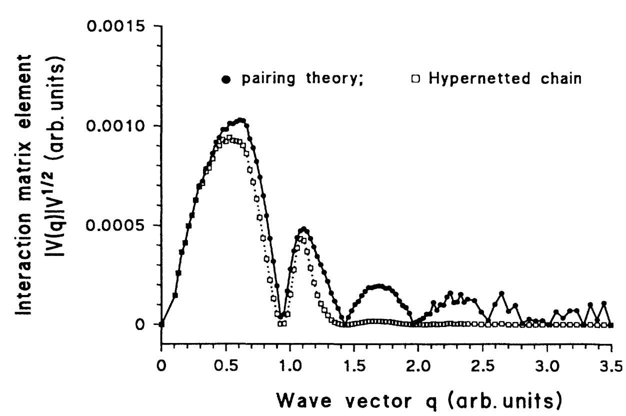

FIG. 1. $|V(q)\sqrt{V}|$ from Eq. (2) from the Bogoliubov pairing theory and from the HNC, using the experimental structure factor of Ref. 10.

The interaction matrix element as discussed here should not be applied for other than ^{3}He atoms in superfluid ^{4}He, like, e.g., the spinning "snowball"[12] where a different type of interaction should be introduced.

Once the polaron model for the ^{3}He interaction with the boson excitations is established and molded into the structure of the Fröhlich Hamiltonian, the powerful calculation techniques of the polaron problem become available to calculate the ground-state energy and the effective mass of ^{3}He. This is of particular interest for the effective mass, because polaron theory allows us to take all self-correlations of the particle into account in an accurate way. In standard notation, an upper bound for the ground-state energy of the model is given by[13]

$$E = \frac{3\hbar}{4}\frac{(v-w)^2}{v} - \sum_{\mathbf{k}} |V(k)|^2 \int_0^\infty d\tau \exp\left(-\hbar\omega(k)\tau - \frac{\hbar^2 k^2}{2m_3}\varphi(\tau)\right), \tag{5}$$

$$\varphi(\tau) \equiv \frac{w^2}{v^2}\tau + \frac{(v^2-w^2)}{\hbar v^3}\left(1 - e^{-\tau\hbar v}\right), \tag{6}$$

in which v and w are variational parameters, to be determined by minimizing the energy expression (5). (For simplicity in the notations, we here only consider the limit of zero temperature, but the extension to the variational calculation of the free energy is straightforward.) These parameters can then be used to calculate the ^{3}He effective mass M_F with the Feynman approach:[13]

$$\frac{M_F}{m_3} = 1 + \frac{2}{3}\sum_{\mathbf{k}} |V(k)|^2 \frac{\hbar^2 k^2}{2m_3} \int_0^\infty d\tau \tau^2 \exp\left(-\hbar\omega(k)\tau - \frac{\hbar^2 k^2}{2m_3}\varphi(\tau)\right). \tag{7}$$

Since $v \rightarrow w$ in the small coupling limit, the effective mass M_p of ^{3}He in superfluid ^{4}He from second-order perturbation theory can be obtained by taking the limit $v \rightarrow w$ in Eq. (7). In terms of the effective Feynman mass one then obtains

$$\frac{M_p}{m_3} = \frac{1}{2 - M_F/m_3}. \tag{8}$$

By the standard conversion of the summation into an integral, the expression (7) for the effective mass M_F is readily written in the form

$$\frac{M_F}{m_3} = 1 + \int_0^\infty dk\, \mu(k). \tag{9}$$

The function $\mu(k)$ as plotted in Fig. 2 reveals that relatively large wave vectors (i.e., larger than the wave vector of about 1 a.u. at the roton minimum in the dispersion relation of the ^{4}He excitations) have a negligible contribution to the effective mass. This feature stresses the importance of an interatomic potential which consistently describes both the static structure factor and the energy of the superfluid for relatively small wave vectors, as realized in the HNC approximation.

The self-energy obtained from Eq. (5) should not be confused with the binding energy of a ^{3}He atom in superfluid ^{4}He, which is the energy required to replace the ^{3}He atom by a ^{4}He atom. This calculation would require an extra term in the Hamiltonian to account for the energy gained if the ^{4}He atom which replaces the ^{3}He is added to the superfluid medium. This interaction term of the ^{4}He atom with the superfluid excitations is absent in the present model.

The minimization of the ^{3}He self-energy (5) has to be performed numerically. Details on the calculation of the variational parameters and of the effective mass with several models will be published elsewhere.

From the Bogoliubov pairing model, i.e., by using $U_{\text{pairing}}(q)$ from Eq. (3), and with the energy of the excitations derived from the experimental structure factor via the Feynman-Bijl relation, one obtains a ^{3}He effective mass of $1.5724m_3$. Since backflow is neglected in the pairing theory, it is not surprising that the ^{3}He effective mass obtained is in good agreement with the effective mass from a hard-core model. Incidentally, if one would assume second-order perturbation theory to be applicable, fortuitous agreement is obtained between the effec-

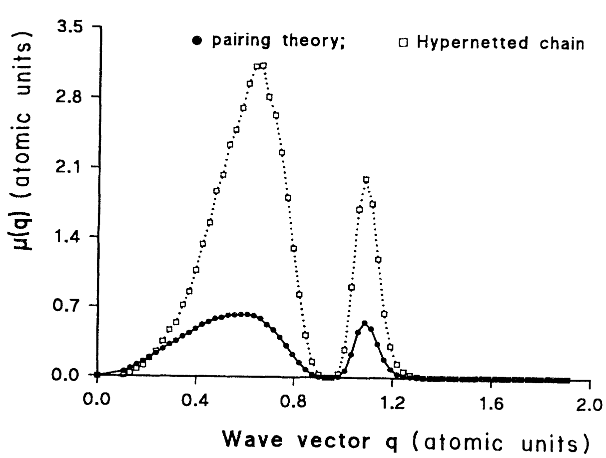

FIG. 2. $\mu(q)$ from Eq. (9) from the Bogoliubov pairing theory and from the HNC, using the experimental structure factor of Ref. 10.

tive mass of $2.335m_3$ from Eq. (8) and the experimental mass. Since the excitation energies from the Feynman-Bijl relation are not in quantitative agreement with their experimental spectrum, the question arises what is the effect of using the experimental boson frequencies in the calculation of the ^{3}He effective mass. If the internal consistency of the Bogoliubov pairing model is thus relaxed by violating the Feynman-Bijl relation, a ^{3}He effective mass of $4.3968m_3$ is obtained. The effective mass is thus quite sensitive to the details and the internal consistency of the model, and the pairing theory seems not appropriate for an accurate quantitative calculation of the effective mass.

As discussed above, the interatomic potential from the HNC approximation provides a quantitatively more accurate framework for the description of superfluid ^{4}He and of ^{3}He in ^{4}He. This is also confirmed by the calculation of the ^{3}He effective mass from the polaron model which we propose in this paper. Using the interatomic potential $U_{\mathrm{HNC}}(q)$ of Eq. (4) in the matrix elements $V(q)$ [see Eq. (2)] of the interaction term between the ^{3}He atom and the boson field in the Fröhlich Hamiltonian, we obtain a ^{3}He effective mass of $2.3121m_3$, to be compared with the experimental effective mass of $2.3m_3$.

The main result of this paper is the derivation of a polaronlike model for the accurate description of a ^{3}He atom in superfluid ^{4}He. The matrix elements $V(q)$ for the interaction between the ^{3}He atom and the superfluid excitations require the knowledge of the interatomic interaction potential $U(q)$ between the atoms in the mixture. It is important that the interatomic potential adequately describes both the experimental structure factor and the experimental excitation spectrum of superfluid ^{4}He in the long wavelength limit, like, e.g., in the HNC approach. Qualitative agreement—as with the Bogoliubov pairing theory—is not sufficient. Second-order perturbation theory is inappropriate for calculating the ^{3}He effective mass, as is also recognized in the HNC approach,[5] where one should use a wave function which at least involves three-particle correlations. These higher-order correlations are variationally included by applying Feynman's path-integral treatment of the polaron model (generalized for frequency-dependent boson excitations), as is confirmed by the very satisfactory calculation of the ^{3}He effective mass in superfluid ^{4}He.

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