Theory of the excitation spectrum of liquid ^{4}He

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A critical review of the theory of a Bose liquid at $T = 0$ as given by Beliaev, Hugenholtz, and Pines and by Brueckner and Sawada is presented. An improved solution of Brueckner's nonlinear integral equation for the vertex functions is proposed. Such a solution is based on a proper parametrization of the angular-momentum dependence of the Green's function. The experimental excitation spectrum is very well reproduced by the theory in the range of linear momenta $0 \leq q \leq 2.3$ Å^{-1}. Remarkably, the calculated density is in exact accord with the experimental value.

The theory of liquid ^{4}He at $T=0$ as proposed by Beliaev[1,2] and subsequently improved, among others, by Hugenholtz and Pines[3] is closely connected with quantum field theory. To start with, the one-particle Green's function, defined, in the interaction representation, as a time-ordered product of the boson fields $\psi(x)$, $\psi^\dagger(x)$ and the S matrix,

$$iG(x-x') = \langle T\{\psi(x)\psi^\dagger(x')S\}\rangle/\langle S\rangle \ , \qquad (1)$$

is considered.

In (1) the expectation value is taken in the ground state of the noninteracting particles which has all the particles in the condensed phase ($N_{\vec{p}\neq 0}=0$, $N_0=N$, N being the number of particles).

In order to take properly into account the depletion of the condensed phase, due to the interaction, Beliaev splits (1) into two parts to describe the propagation of a particle in and outside the zero-momentum state, respectively. The former is evaluated exactly, while the latter Green's function obeys an equation entirely analogous to the one originally proposed by Dyson[4] in quantum electrodynamics.

The solution can be given exactly in terms of three vertex functions, customarily denoted $\Sigma_{11}(p)$, $\Sigma_{02}(p+\mu)$, and $\Sigma_{20}(p+\mu)$, and of the chemical potential μ and reads (p is the four-momentum of the particle)

$$G(p+\mu) = \frac{p^0+\epsilon^0_{\vec{p}}+\Sigma^-_{11}-\mu}{[p^0-\frac{1}{2}(\Sigma^+_{11}-\Sigma^-_{11})]^2-[\epsilon^0_{\vec{p}}+\frac{1}{2}(\Sigma^+_{11}+\Sigma^-_{11})-\mu]^2+\Sigma_{20}\Sigma_{02}+i\delta} \ , \qquad (2)$$

where $\epsilon^0_{\vec{p}}=\vec{p}^2/2m$ and $\Sigma^\pm_{11}=\Sigma_{11}(\pm p)$.

The poles of $G(p+\mu)$ near the real p^0 axis give the energies of a quasiparticle of momentum $\vec{p}$.

To proceed further the vertex functions, i.e., the irreducible parts in the expansion of the Green's function, must be determined. Of these $\Sigma_{11}(p)$ describes the process of the forward scattering of a particle outside the condensate with a zero-momentum particle, while $\Sigma_{02}(p+\mu)$ and $\Sigma_{20}(p+\mu)$ describe the absorption into and the emission from the condensed phase of two particles.

Therefore one sees that the Dyson equation does not allow for the free propagation of the Helium atoms: on the contrary, the interaction with the condensed medium is always present.

The vertex functions can be obtained, with a proper specification of the variables, from the so-called "effective potential" $\Gamma(12,34)$ which in Beliaev's theory obeys the following integral equation:

$$\Gamma(12;34) = U(1-2)\delta(1-3)\delta(2-4) + i\int U(1-2) \times G^0(1-5)G^0(2-6)\Gamma(56;34)\, d^4x_5\, d^4x_6 \ , \qquad (3)$$

where U is the interaction potential and $G^0=(p^0-\epsilon^0_{\vec{p}}+i\delta)^{-1}$ is the *free* one-particle Green's function.

Equation (3) sums up all the ladder diagrams of

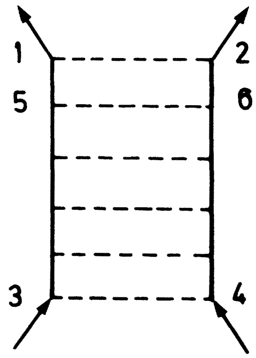

FIG. 1. One of the many ladder diagrams summed up in Eq. (3).

the type illustrated in Fig. 1. We emphasize that the particles propagate freely, with momentum different from zero, from one vertex to another along the borders of the ladder. This is inconsistent with the original equation for $G(p+\mu)$, where the propagation of the particles with nonvanishing momentum is always affected, as already noted, by the interaction with the zero-momentum particles.

The solution of Eq. (3) can be expressed in terms of the two-body scattering amplitude $f(\vec{p}'; \vec{p})$ in vacuum [the quantity $f(\vec{p}'; \vec{p})$ becomes the usual scattering amplitude (apart from a factor -4π) when $|\vec{p}'| = |\vec{p}|$] as follows:

$$\Gamma(\vec{p}'; \vec{p}; P) = f(\vec{p}', \vec{p}) + \int d\vec{q}\, f(\vec{p}', \vec{q}) f^*(\vec{p}, \vec{q}) \times \left(\frac{1}{K_0^2 - q^2 + i\delta} - \frac{1}{p^2 - q^2 + i\delta} \right), \quad (4)$$

where $\vec{p}$ and $\vec{p}'$ are the relative initial and final momenta of the two interacting particles, P is the total four-momentum of the interacting pair, and $K_0^2 = P^0 - \frac{1}{4}\vec{P}^2$.

If only the first term in the right-hand side of Eq. (4) is retained [this is *not* just the first iteration of Eq. (3)], then one gets immediately for the excitation spectrum

$$\omega(\vec{p}) = \{[\epsilon_{\vec{p}}^0 + 2n_0 f_s(\tfrac{1}{2}\vec{p}, \tfrac{1}{2}\vec{p}) - n_0 f(0,0)]^2 - n_0^2 |f(\vec{p}, 0)|^2\}^{1/2}, \quad (5)$$

where the symmetrized scattering amplitude is defined by

$$f_s(\vec{p}', \vec{p}) = \tfrac{1}{2}[f(\vec{p}', \vec{p}) + f(-\vec{p}', \vec{p})], \quad (5')$$

and n_0 is the density of the condensed phase, which appears here explicitly because of the previously mentioned separation of the one-body Green's function (1) into two parts.

Formula (5) actually is quite general and holds whenever the p^0 dependence of the vertex functions can be ignored. Beliaev[2] then considers the model of a gas of hard spheres of radius $\frac{1}{2}a$. Keeping only the s-wave interaction, (5) becomes ($p = |\vec{p}|$):

$$\omega(p) = (6.06/a^2)\{[x^2 + 6\beta(3\sin x/x - 1)] \times [x^2 + 6\beta(\sin x/x - 1)]\}^{1/2}, \quad (6)$$

where $x = pa$, $\beta = n_0(\frac{4}{3}\pi a^3)$, and the factor 6.06 is to convert from units of Å^{-2} to °K. Formula (6) cannot reproduce the experimental data. The sound velocity associated with Eq. (6) is

$$c = (6.06/a)(12)^{1/2}[\beta(1-\beta)]^{1/2}. \quad (7)$$

So when the density of the condensed phase becomes larger than $\frac{1}{8}$ of the close-packing density $\rho_{cp}(=6/\pi a^3$ for hard spheres of radius $\frac{1}{2}a)$ no phonons will propagate into the system. Also the maximum value of c given by (7) (corresponding to $\beta = \frac{1}{2}$) is 5.25 °K Å (with $a \approx 2$ Å), to be compared with the commonly accepted experimental value of 18.3 °K Å.

We believe these shortcomings of the Beliaev theory to be mostly due to the lack of self-consistency, rather than to the approximations made in solving Eq. (4) or to the neglect of the interaction in higher partial waves.

When viewed in the framework of this formalism, Brueckner's theory[5,6] amounts essentially to the use of a more realistic integral equation for the vertex functions in order to deal better with the problem of the propagation of the particles with nonvanishing momentum.

In fact in Brueckner's theory the excitation spectrum is given by a formula identical to (5) but with the "t matrix" in place of the two-body free scattering amplitude, i.e.,

$$\omega(q) = \{[q^2/2m + N(t_{0q,0q} + t_{0q,q0} - t_{00,00})]^2 - N^2 t_{00,q-q}^2\}^{1/2}. \quad (8)$$

The suffix zero labels atoms in the condensate, and N is the number of particles. Since (8) involves N, while (5) has n_0, Brueckner theory does not explicitly take into account the depletion of the condensate. This depletion will occur in higher-order terms, together with the contributions of the particles excited out of the condensate. This seems physically reasonable.

The integral equation for the t matrix is now

$$t_{12,34} = U_{12,34} + U_{12,56} G_{56} t_{56,34}, \quad (9)$$

where, in the two-body propagator

$$G(q) = -\{2[q^2/2m + N(t_{0q,0q} + t_{0q,q0} - t_{00,00})] + i\delta\}^{-1}, \quad (10)$$

the interaction with the particles in the condensed medium is taken into account through the explicit self-consistency term $N(t_{0q,0q}+t_{0q,q0}-t_{00,00})$. In terms of diagrams, the particles on the border of the ladder of Fig. 1 are now allowed to interact an infinite number of times with the zero-momentum particles.

As a result the integral equation (9) becomes highly nonlinear, the price to be paid to account for higher-order diagrams neglected in Beliaev's treatment.

The question then arises if these higher-order processes are the important ones to be considered. One may try to answer this question by comparing the theory with experiment, having first solved Eq. (9).

If an infinite hard-core two-body potential is used then scattering theory[2] gives

$$t(q)\equiv t_{0q,0q}+t_{0q,q0}-t_{00,00}$$
$$=-2\sum_{l\text{ even}}(2l+1)\frac{j_l^2(\frac{1}{2}qa)}{G_l(a,a)}+\frac{1}{G_0(a,a)} \qquad (11)$$

and

$$t_{00,q-q}=[-1/G_0(a,a)]\sin(qa)/qa\ , \qquad (12)$$

where the $G_l(a,a)$, the lth partial waves of the two-body Green's function in configuration space, are still unknown. The j_l's are the standard spherical Bessel functions.

Assuming, as Brueckner does, $G_l(a,a)=G_0(a,a)$, the expansion (11) can readily be summed:

$$t(q)=-[1/G_0(a,a)]\sin(qa)/qa\ . \qquad (13)$$

The resulting spectrum is quite simple because of the exact cancellation of the quadratic terms in (8):

$$\omega(q)=6.06q\left(q^2+2\frac{\lambda^2}{a^2}\frac{\sin(qa)}{qa}\right)^{1/2}\ , \qquad (14)$$

where $\lambda^2=-Na^2/G_0(a,a)$ and $\hbar^2=2m=1$. The corresponding sound velocity is $c=6.06\lambda\sqrt{2}/a$.

Equation (14) displays the roton minimum for λ large enough and has the correct analytic properties,[7] i.e., branch cuts in the complex q plane with the real part set by the roton minimum and imaginary part decreasing as the density becomes larger.

These features indicate that Brueckner's theory indeed contains the essential dynamical aspects of liquid ^{4}He. Nevertheless it has been shown[8] that (14), as it stands, cannot quantitatively reproduce the experimental data with any choice of a and λ^2.

In order to obtain a better solution of Eq. (9) we relaxed the crude approximation $G_l=G_0$, which strongly underestimates the contribution of the higher partial waves to the t matrix and conjectured for all the waves higher than $l=0$,

$$G_l(a,a)=G_0(a,a)/A(l^2+l+1)\ , \qquad (15)$$

which permits a closed analytic expression for the summation (11), i.e.,

$$Nt(q)=\delta\{(1-A)[1-2j_0^2(\tfrac{1}{2}qa)]-\tfrac{1}{2}A[j_0(qa)+\cos(qa)+\tfrac{1}{3}(qa)^2]\}\ . \qquad (16)$$

Inserting (16) and (13) into (8), one gets

$$\omega(q)=6.06\Big[\big(q^2+\delta\{(1-A)[1-2j_0^2(\tfrac{1}{2}qa)]-\tfrac{1}{2}A[j_0(qa)+\cos(qa)+\tfrac{1}{3}(qa)^2]\}\big)^2-\delta^2j_0^2(qa)\Big]^{1/2}\ , \qquad (17)$$

where $\delta=N/G_0(a,a)$.

The experimental data[9] in the range $0\leq q\leq 2.3$ Å^{-1} are now reproduced exceedingly well for the values

$$\delta=-5.483\ \text{Å}^{-2},\quad a=2.019\ \text{Å},\quad A=0.071\ , \qquad (18)$$

as can be seen from Table I and Fig. 2. The corresponding χ^2 is 9.415, which is entirely acceptable for a three-parameter fit to 23 data points.

Incidentally, Eq. (17) provides the same sound velocity, namely $c=6.06(-2\delta)^{1/2}$, as Eq. (14). The

TABLE I. Dispersion curve in liquid ^{4}He given by our Eqs. (17) (column IV) and (24) (column V) compared with the experimental points of Ref. 5.

Wave vector q (Å^{-1})	Expt. energy (°K)	Error	Theor. I	Theor. II
0.2	3.700	0.50	3.956	3.956
0.3	5.650	0.20	5.829	5.828
0.4	7.400	0.20	7.577	7.576
0.5	9.150	0.20	9.165	9.164
0.6	10.750	0.20	10.559	10.559
0.7	11.750	0.20	11.734	11.733
0.8	12.650	0.20	12.667	12.666
0.9	13.150	0.20	13.341	13.340
1.0	13.550	0.25	13.749	13.748
1.1	13.800	0.30	13.887	13.886
1.2	13.750	0.25	13.762	13.761
1.3	13.500	0.25	13.388	13.386
1.4	12.950	0.20	12.791	12.789
1.5	12.200	0.20	12.010	12.008
1.6	11.200	0.20	11.109	11.108
1.7	10.250	0.20	10.184	10.184
1.8	9.250	0.20	9.385	9.389
1.9	8.700	0.20	8.923	8.931
2.0	8.950	0.20	9.037	9.047
2.1	10.000	0.20	9.883	9.889
2.2	11.650	0.25	11.459	11.449
2.3	13.550	0.25	13.650	13.612

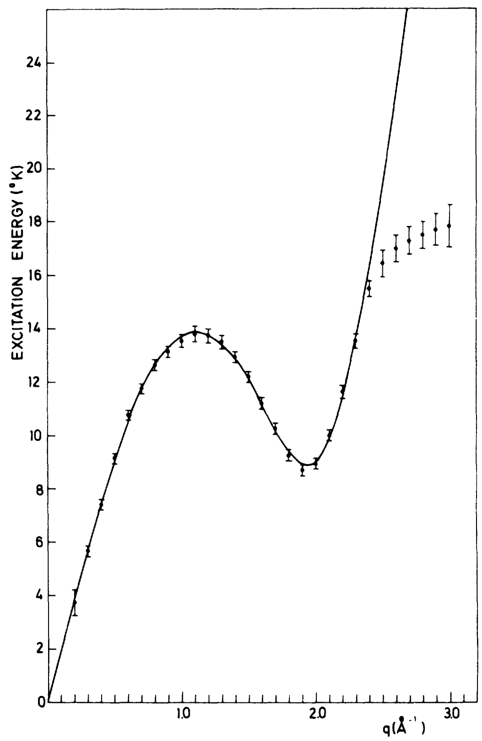

FIG. 2. Dispersion curve in liquid ^{4}He as given by our formula (17) (solid line) compared with the experimental data taken from Cowley and Wood (Ref. 9).

radius of the hard core, even if somewhat small, is reasonable.

The propagator (10) is the distinguishing feature of Brueckner's theory. Its poles near the real axis in the complex ω plane fail to give the quasiparticle spectrum because of the presence of the extra term $N^2 t^2_{00,q-q}$ under the square root in (8). This term describes the multiple excitation of pairs of particles out of the condensed phase, as illustrated diagrammatically in Fig. 3, and its inclusion is essential for a proper description of the excitation spectrum.

To test the choice (10) and therefore, in a sense, the validity of Brueckner's theory, we consider

$$G_0(a,a)=\frac{\Omega}{(2\pi)^3}\int d\vec{q}\,\frac{\sin^2(qa)}{(qa)^2}\,G(q)\;, \tag{19}$$

where Ω is the volume and

$$G(q)=-\tfrac{1}{2}[q^2+N(t_{0q,0q}+t_{0q,q0}-t_{00,00})]^{-1}\;. \tag{20}$$

From (19) and (20) one gets

$$\rho a^3=-\frac{\delta}{(2\pi)^2}\times\int_0^\infty dx\,\frac{\sin^2 x}{\{[\omega(q)/6.06]^2+N^2t^2_{00,-qq}\}^{1/2}}\;, \tag{21}$$

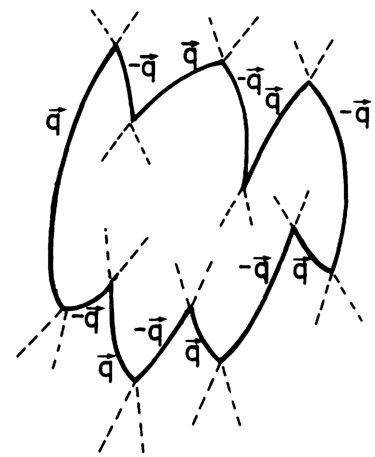

FIG. 3. Typical multiple-excitation diagram. Note that only one value of q is involved. Dashed lines represent particles in the condensate.

$$\rho a^3=\frac{\lambda^2}{(2\pi)^2}\int_0^\infty dx\,\frac{\sin^2 x}{\{[a^2\omega(q)/6.06]^2+\lambda^4 j_0^2(x)\}^{1/2}}\;, \tag{21'}$$

which, with the values (18) for δ, a, and A, gives for the density (1/45.8) Å^{-3}, in *exact accord* with the experimental value. This connection between the density and the excitation spectrum is specific to the Brueckner theory, with its explicit self-consistency term in $G(q)$.

So with the correct $\omega(q)$ one gets the right density from (21′): a strong indication that multiple excitations and self-consistency are quite relevant and correctly handled in Brueckner's theory. The exact agreement with the experimental density also justifies ignoring the depletion of the condensate.

In Fig. 4 the quantity $\lambda^2=-\delta a^2$ is displayed as a function of ρa^3: it appears that the sound velocity (proportional to λ) increases with the density up to a maximum value $c_{\max}\cong 30$ °K Å which is reached when $\rho a^3\approx 6/\pi$.

This behavior is radically different from (7). In the complex q plane the relevant singularities of (8) are branch points located at $q=q_1\pm iq_0=1.91\pm i0.31$ Å^{-1}, in agreement with the analytic structure found in Ref. 7.

We have also investigated the following conjecture for the partial-wave Green's function (except for $l=0$):

$$G_l(a,a)=G_0(a,a)/A(2l+1)\;. \tag{22}$$

In this case also a closed analytic expression for the summation (11) is obtainable, i.e.,

$$Nt(q)=\delta\{2(A-1)j_0^2(\tfrac{1}{2}qa)+1-\tfrac{1}{2}A[j_0(qa)+\cos(qa)+qa\,\mathrm{Si}(qa)+\pi\mathcal{H}_{-1}(qa)]\}\;, \tag{23}$$

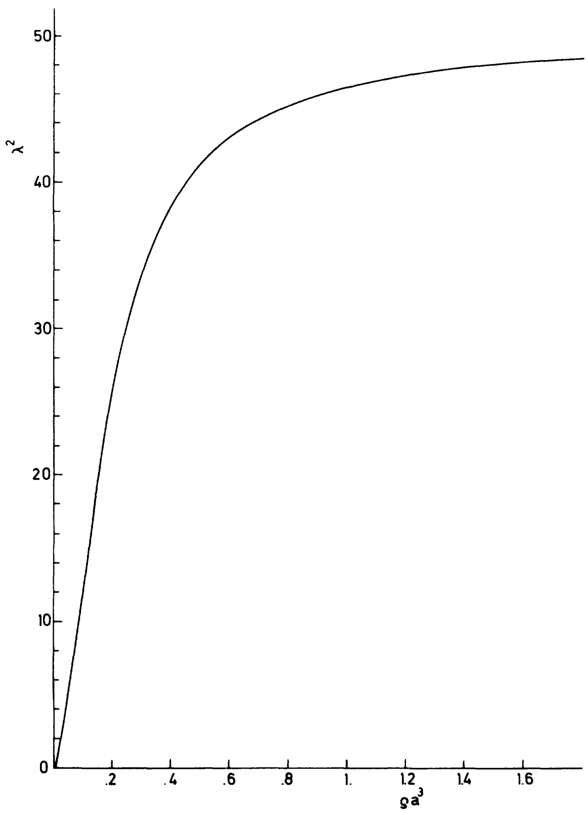

FIG. 4. Solution of Eq. (21′) giving $\lambda^2 = -\delta a^2 = -[N/G_0(a,a)]a^2$ as a function of ρa^3.

where $\mathrm{Si}(qa)$ and $\mathcal{H}_{-1}(qa)$ are, respectively, the sine integral and the Struve function of order -1.[10]

Inserting again (23) and (13) into (8), one gets

$$\omega(q) = 6.06\left[\left(q^2 + \delta\{2(A-1)j_0^2(\tfrac{1}{2}qa) + 1 - \tfrac{1}{2}A[j_0(qa) + \cos(qa) + qa\,\mathrm{Si}(qa) + \pi\mathcal{H}_{-1}(qa)]\}\right)^2 - \delta^2 \sin^2(qa)/(qa)^2\right]^{1/2} . \quad (24)$$

From Table I it is seen that the experimental data can be reproduced very well ($\chi^2 = 9.540$) in the range $0 \leq q \leq 2.3$ Å^{-1} for the values

$$\delta = -5.482\ \text{Å}^{-2}, \quad a = 2.021\ \text{Å}, \quad A = 0.101 . \quad (25)$$

Note that (24) provides the same sound velocity as (17), namely $c = 6.06(-2\delta)^{1/2}$. Also, inserting (24) with the values (25) in (21′) one gets again the experimental density.

The value (25) for A is larger than the value (18), as it should be since the ansatz (22) emphasizes less drastically the role of the higher partial waves. The branch points characterizing (24) coincide with those of Eq. (17).

Even if a theoretical deduction of the link between $G_l(a,a)$ and $G_0(a,a)$ is difficult to achieve in general, one may proceed as follows. From the partial-wave decomposition of the Green's function

$$G_l(r, r') = \tfrac{1}{2}\int_{-1}^{+1} d\mu\, P_l(\mu) G(\vec{r} - \vec{r}') , \quad (26)$$

where the $P_l(\mu)$ are the Legendre polynomials, taking the simplest expression

$$G(\vec{r} - \vec{r}') = -\frac{m\Omega}{4\pi}\frac{e^{-|\vec{r}-\vec{r}'|(8\pi\rho a)^{1/2}}}{|-\vec{r} - \vec{r}'|} , \quad (27)$$

after some nontrivial manipulations one gets

$$G_l(a,a) = -\frac{m\Omega}{4\pi a} I_{l+1/2}(8\pi\rho a^3)^{1/2} K_{l+1/2}(8\pi\rho a^3)^{1/2} , \quad (28)$$

where $I_{l+1/2}$ and $K_{l+1/2}$ are the Bessel functions of purely imaginary argument of first and second kind, respectively. Exploiting their asymptotic representation we get

$$G_l(a,a) \cong 2G_0(a,a)/(2l+1) , \quad (29)$$

which supports the ansatz (22).

Our analysis suggests that off-energy-shell effects and the phonon-phonon interaction do not play a significant role in the excitation spectrum of liquid ^{4}He.

The intermediate-range attraction, neglected in the present treatment, seems to be of importance only in the low-q region, as can be argued from the fact that our sound velocity $c = 20.1 \div 20.2$ °K Å is about 10% larger than the experimental value 18.3 °K Å. This discrepancy can be accounted for by attractive forces, as discussed in Ref. [8].

Of course attractive forces are essential for the binding energy of the system (7 °K per particle). To obtain binding from two-body clusters, $t_{00,00}$ must be negative. But then $\omega(q)$ becomes imaginary for small q, indicating an instability. Therefore, as mentioned by Brandow,[11] three-body and higher clusters should be significant for the binding of liquid ^{4}He.

In conclusion our analysis shows that an accurate solution of Eq. (9) is most essential for a proper account of the liquid ^{4}He dispersion relation. It is also remarkable that if the fit to the experimental data is extended to higher values of q, then already for $q_{max} = 2.4$ Å^{-1} one gets a sensible worsening of the χ^2(= 14.2); an indication that some new elements come into play, in particular, a possible hybridization with the two-roton branch.[12]

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