where we have made use of the identity[12]

$$\Gamma(a)\Gamma(1-a)=\pi/\sin\pi a.$$

Now

$$\sin(\pi/2+i\gamma\pi/2p)=\cosh(\gamma\pi/2p)$$

so

$$e^{-ipr/2}{}_1F_1(\tfrac{1}{2}+i\gamma/2p;1;ipr)$$
$$=\frac{\cosh(\pi\gamma/2p)}{\pi}\int_0^1\frac{e^{ipr(t-\frac{1}{2})}}{[t(1-t)]^{1/2}}\left(\frac{t}{1-t}\right)^{i\gamma/2p}dt. \qquad \text{(C3)}$$

Letting $u=1-t$; $du=-dt$; $t-\frac{1}{2}=\frac{1}{2}-u$ (C3) becomes

$$e^{-ipr/2}{}_1F_1(\tfrac{1}{2}+i\gamma/2p;1;ipr)$$
$$=\frac{\cosh(\pi\gamma/2p)}{\pi}\int_0^1\frac{e^{ipr(\frac{1}{2}-u)}}{[u(1-u)]^{1/2}}\left(\frac{1-u}{u}\right)^{i\gamma/2p}du$$
$$=\frac{\cosh(\gamma\pi/2p)}{\pi}\int_0^1\frac{e^{-ipr(u-\frac{1}{2})}}{[u(1-u)]^{1/2}}\left(\frac{u}{1-u}\right)^{-i\gamma/2p}du. \qquad \text{(C4)}$$

Comparing the right-hand sides of Eqs. (C3) and (C4), we see that $e^{-ipr/2}{}_1F_1(\frac{1}{2}+i\gamma/2p;1;ipr)$ is also equal to its complex conjugate, hence it is real. Thus, the eigenfunctions $R(\lambda_k,\gamma,r)$ are real.

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[12] Reference 6, Chap. 6, p. 256, formula (6.1.17).

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Excitation Spectrum of the Bose Liquid

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The assumptions and predictions of the Brueckner-Sawada method (including recent refinements) for the derivation of the excitation spectrum of the high-density boson system are examined using Green's-function techniques and a new method of solving the scattering-matrix equation. In the case of the real interaction potential of He^4 atoms, the spectrum obtained in our approximation has the correct form but the depletion has a meaningless value. It is pointed out that a probable cause of discrepancies is inconsistent omission of certain self-energy terms.

INTRODUCTION

THERE are several microscopic approaches to the derivation of the excitation spectrum of the zero-temperature boson system,[1] which have been used to derive the phonon part of the spectrum. To obtain the roton minimum, methods for a nondilute gas must be used. Some clarification of the reason for the appearance of the roton dip was already given by the argument of Feynman[2] showing connection between quasiparticle energy $\epsilon(k)$ and the liquid-structure function $S(k,\omega)$. The purely microscopic derivations have concentrated almost exclusively on the case of hard-sphere bosons. Brueckner and Sawada[3] (BS) treated the hard core as a screened delta-function potential, and found qualitative agreement with the Landau curve. Parry and ter Haar[4] found that the roton minimum disappears if the depletion effect is included in these calculations. Even poorer agreement was found when an attractive tail was added to the hard core, and they concluded that the hard-sphere boson gas is not as good a model for liquid helium as has been assumed. Liu, Liu, and Wong[5] showed, however, that a qualitatively correct excitation spectrum is found if, instead of this treatment, the hard-sphere potential is replaced by the two-body pseudopotential earlier considered by Lee, Huang, and Yang.[6]

The approach used in the quoted papers is called the Brueckner-Sawada method. Because it still forms one of the main efforts to microscopic derivation of the excitation spectrum of liquid helium II, we consider it worthwhile to study some aspects of the approximations and predictions of the theory. In the next two sections the quasiparticle spectrum, the depletion, and the reaction matrix equation are derived using Green's-function techniques at zero temperature. The BS method is then shown to have the following properties: [1] The quasiparticle energy is assumed to be given by the poles of the single-particle Green's function. [2] In this, only the self-energy resulting from first-order terms of the effective interaction with the particles in the condensate is included. [3] The effective interaction is given by the BS equation for the scattering matrix, in which the propagator between successive

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[1] For review, see, e.g., P. C. Hohenberg and P. C. Martin, Ann. Phys. (N. Y.) **34**, 291 (1965).

[2] R. P. Feynman, Phys. Rev. **91**, 1301 (1953); **94**, 262 (1954); R. P. Feynman and M. Cohen, *ibid.* **102**, 1189 (1956).

[3] K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 1117 (1957); **106**, 1128 (1957).

[4] W. E. Parry and D. ter Haar, Ann. Phys. (N.Y.) **19**, 496 (1962).

[5] L. Liu and K. W. Wong, Phys. Rev. **132**, 1349 (1963); L. Liu, Lu Sun Liu, and K. W. Wong, *ibid.* **135**, A1166 (1964).

[6] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).

scatterings is taken to be the above Green's function, except that [4] here in addition the process of a pair of particles scattering into, or out of, the condensate is neglected. [5] The center-of-mass approximation is adopted throughout.

Predictions of the equations are considered in the remaining sections. We first develop a method to solve a T-matrix equation of the BS type. By expanding in spherical harmonics, the equation can be transformed into a set of integral equations in one real variable. After partially transforming into coordinate space these equations can be solved numerically in a straightforward manner. In contrast to previous calculations this procedure is applicable to any interaction potential.

The excitation spectrum and the depletion are calculated for hard spheres and for the experimentally and theoretically well-known interaction potential of He^4 atoms. The behavior of the spectrum including the roton dip agrees semiquantitatively with the neutron diffraction data. The depletion, however, turns out to have a meaningless value and is inconsistent with a value used elsewhere in the approximation scheme.

Several conclusions on the validity of the approach can be drawn. The assumption [1] is valid because, as shown by Hohenberg and Martin,[1] in a condensed Bose system the single-particle propagator and the density-correlation function (relating to scattering) have the same poles. The BS scheme of evaluating the positions of the poles presumably has some meaning for a nondilute gas as it gives the roton modes, which are absent in low-density calculations using the free-particle propagator in the T-matrix equation. The inconsistencies in the values of the depletion for liquid-helium density, however, show the inadequacy of the theory. The largest part of the error presumably comes from [4], which has the effect of replacing the phonon spectrum by an energy gap, and also causes the inconsistency of using different self-energy expressions in the T-matrix and excitation spectrum calculations.

THE GREEN'S FUNCTION AT ZERO TEMPERATURE

In the formalism of Beliaev[7] the operators referring to particles in $k\neq 0$ states and those referring to particles in the condensate are separated. There are then two kinds of propagators: those for $k\neq 0$ are denoted by $G^{(0)}(x-x')$ and by a straight line, and those for $k=0$ by a zigzag line. The diagram describing a self-energy part of a particle not in the condensate will contain two external straight lines and in addition an even number of zigzag lines stemming from the interaction of particles not in the condensate with particles in the condensate. There are now three different types of self-energy diagrams: (a) diagrams with one ingoing and one outgoing straight line, and with n ingoing and n outgoing zigzag lines ($n=0, 1, \cdots$). The sum of irreducible self-energy parts of this type is denoted by $\Sigma_{11}(x-x')$. (b) Diagrams with two outgoing straight lines, $n+2$ ingoing, and n outgoing zigzag lines. The sum of irreducible self-energy parts is $\Sigma_{02}(x-x')$. (c) Diagrams with two ingoing straight lines, n ingoing and $n+2$ outgoing zigzag lines. The sum of irreducible self-energy parts is $\Sigma_{20}(x-x')$.

The analog Dyson's equation is a set of two equations. Solving, one finds for the exact Green's function of a particle not in the condensate the momentum space expression

$$G'(p)=\frac{\omega+\epsilon_0(\mathbf{p})+S(p)-A(p)-\mu}{(\omega-A(p))^2-(\epsilon_0(\mathbf{p})+S(p)-\mu)^2+\Sigma_{20}(p)\Sigma_{02}(p)+i\delta}, \tag{1}$$

with the notation

$$S(p)=\tfrac{1}{2}(\Sigma_{11}(p)+\Sigma_{11}(-p)),\ A(p)=\tfrac{1}{2}(\Sigma_{11}(p)-\Sigma_{11}(-p)),\ \epsilon_0(\mathbf{p})=\mathbf{p}^2/2m.$$

The equations have been written for the grand canonical ensemble with μ as a free variable.

The excitation spectrum is given by the poles of $G'(p)$,

$$\omega=A(p)+\{[\epsilon_0(p)+S(p)-\mu]^2-\Sigma_{20}(p)\Sigma_{02}(p)\}^{1/2}, \tag{2}$$

where the square root must be taken with positive sign. Generally this is an implicit equation for the fourth component ω of p. Later we will work in an approximation in which the self-energy parts $\Sigma(p)$ do not depend on ω, and thus the quantity (2) is directly $\epsilon(\mathbf{p})$.

In the presence of interaction the number density of the particles in the condensate n_0 is different from the total number density $n=N/\Omega$. The depletion is given by the number of particles not in the condensate,

$$n-n_0=\lim_{t'\to t+0} iG'(x-x'),\qquad \mathbf{x}=\mathbf{x}'.$$

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[7] S. T. Beliaev, Zh. Eksperim. i Teor. Fiz. 34, 417 (1958); 34, 433 (1958) [English transls.: Soviet Phys.—JETP **7**, 289 (1958); **7**, 299 (1958)]; see A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).

In momentum space this becomes

$$n-n_0=\lim_{t\to 0+} i\int \frac{d^3p}{(2\pi)^3}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}G'(\mathbf{p},\omega)e^{i\omega t}=i\int\frac{d^3p}{(2\pi)^3}\int_C\frac{d\omega}{2\pi}G'(\mathbf{p},\omega),$$

where the contour C is the real axis closed by a large semicircle in the upper half-plane. We again assume that the self-energy parts $\Sigma(p)$ do not depend on ω. Substitution of Eq. (1) and evaluation of the residue at the pole in the upper half-plane gives

$$n-n_0=\int\frac{d^3p}{(2\pi)^3}\frac{S(\mathbf{p})+\epsilon_0(\mathbf{p})-\mu-\{[S(\mathbf{p})+\epsilon_0(\mathbf{p})-\mu]^2-\Sigma_{20}(\mathbf{p})\Sigma_{02}(\mathbf{p})\}^{1/2}}{2\{[S(\mathbf{p})+\epsilon_0(\mathbf{p})-\mu]^2-\Sigma_{20}(\mathbf{p})\Sigma_{02}(\mathbf{p})\}^{1/2}}.$$

It is seen that neglecting the ω dependence of the $\Sigma(p)$:s also means that the poles of $G'(p)$ are assumed to exhaust the whole spectrum of the spectral density function and that the normalization of the resonances does not enter. The numerical results quoted in the last section indicate that the normalization constants in fact may be important.

From symmetry with respect to the sign of p there follows the equation

$$\Sigma_{02}(p)=\Sigma_{20}(p).$$

Further, one can show that at zero temperature the chemical potential is[7]

$$\mu=\Sigma_{11}(0)-\Sigma_{02}(0). \tag{3}$$

This equation can also be derived, apart from the sign of $\Sigma_{02}(p)$, from Eq. (2), assuming that $\epsilon(0)$ vanishes.

THE REACTION MATRIX

To carry out explicit computations some approximation must be chosen for the irreducible self-energy parts Σ. The simplest approximation is to take the first-order terms in the interaction. When the interaction potential $U(x-x')$ has a hard-core part, the matrix elements in momentum space are infinite, and one must use instead the effective potential obtained by summing the multiple scattering diagrams of the two particles over all orders. The resulting scattering matrix is given by the equation

$$\begin{aligned}T(k_1,k_2,k_3,k_4)&=U(\mathbf{k}_3-\mathbf{k}_1)+i\int\frac{d^4p}{(2\pi)^4}U(\mathbf{k}_1-\mathbf{p})G'(p)\\&\quad\times G'(k_1+k_2-p)T(p,\,k_1+k_2-p,\,k_3,\,k_4).\end{aligned} \tag{4}$$

Replacing the interaction potential by the T matrix gives expressions for $\Sigma_{11}(p)$ and $\Sigma_{02}(p)$. Equation (2) gives, then, the quasiparticle energies.

If the free-particle propagator,

$$G^{(0)}(p)=[\omega-\epsilon_0(\mathbf{p})+\mu+i\delta]^{-1},$$

is used for $G'(p)$ in Eq. (4), the results are valid in the low-density limit only. To account for interactions with background particles between successive interactions, one may use for $G'(p)$ the expression (1) in which the functions $\Sigma_{11}(p)$ and $\Sigma_{02}(p)$ are taken to be the first-order terms in T. Equation (4) is then a nonlinear integral equation for T.

Introducing total and relative four-momenta

$$K=k_1+k_2=k_3+k_4,\quad k'=\tfrac{1}{2}(k_1-k_2),\quad k=\tfrac{1}{2}(k_3-k_4),$$

Eq. (4) becomes

$$\begin{aligned}T(k',k;K)&=U(\mathbf{k}'-\mathbf{k})+i\int\frac{d^4p}{(2\pi)^4}\\&\quad\times U(\mathbf{k}'-\mathbf{p})G'(\tfrac{1}{2}K+p)G'(\tfrac{1}{2}K-p)T(p,k;K).\end{aligned} \tag{5}$$

From Eq. (4) it is seen that, because $U(q)$ does not depend on the fourth component of the four-vector q, the only dependence of T on the fourth components is through the fourth component of the total four-momentum K. Equation (5) can then be written in the form

$$\begin{aligned}T(\mathbf{k}',\mathbf{k};K)&=U(\mathbf{k}'-\mathbf{k})\\&\quad+\int\frac{d^3p}{(2\pi)^3}U(\mathbf{k}'-\mathbf{p})G(\mathbf{p};K)T(\mathbf{p},\mathbf{k};K),\end{aligned} \tag{6}$$

with

$$G(\mathbf{p};K)=i\int\frac{d\omega}{2\pi}G'(\tfrac{1}{2}K+p)G'(\tfrac{1}{2}K-p),\quad p=(\mathbf{p},\omega). \tag{7}$$

The calculations are essentially simplified if we adapt the center-of-mass approximation, i.e., assume that in Eq. (6) $G(\mathbf{p};K)$ is independent of K. According to the estimates of Parry and ter Haar[4] this appears not to cause appreciable error. The scattering matrix $T(\mathbf{k}',\mathbf{k})$ is then independent of K, and the self-energy parts,

$$\begin{aligned}\Sigma_{11}(\mathbf{p})&=n_0T(\tfrac{1}{2}\mathbf{p},\tfrac{1}{2}\mathbf{p})+n_0T(\tfrac{1}{2}\mathbf{p},\,-\tfrac{1}{2}\mathbf{p}),\\\Sigma_{20}(\mathbf{p})&=\Sigma_{02}(\mathbf{p})=n_0T(\mathbf{p},0),\end{aligned} \tag{8}$$

do not depend on the fourth component of p. The integration in Eq. (7) can be carried out by closing the part of integration and computing the residues at the poles in the upper half-plane. The result is

$$G(\mathbf{p})=-\frac{2[\epsilon_0(\mathbf{p})+\Sigma_{11}(\mathbf{p})-\mu]^2-\Sigma_{02}{}^2(\mathbf{p})}{4\{[\epsilon_0(\mathbf{p})+\Sigma_{11}(\mathbf{p})-\mu]^2-\Sigma_{02}{}^2(\mathbf{p})\}^{3/2}}. \tag{9}$$

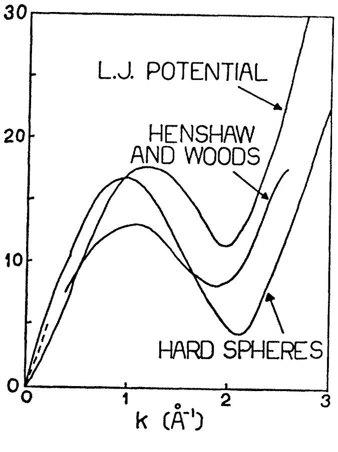

FIG. 1. Calculated excitation spectrum in liquid helium and the experimental curve of Henshaw and Woods.

The value of μ is, according to Eqs. (3) and (8),

$$\mu = n_0 T(0,0).$$

The preceding calculations could be improved by introducing, analogously to the self-energy part, several types of T matrices with n outgoing and $4-n$ ingoing straight lines. The T-matrix equation would then be replaced by a set of equations.

If the self-energy part $\Sigma_{02}(\mathbf{p})$ is neglected in Eq. (9), then

$$G(\mathbf{p}) = -[(\mathbf{p}^2/m) + n_0 T(\tfrac{1}{2}\mathbf{p}, \tfrac{1}{2}\mathbf{p}) + n_0 T(\tfrac{1}{2}\mathbf{p}, -\tfrac{1}{2}\mathbf{p}) - n_0 T(0,0)]^{-1}. \quad (10)$$

Equation (6) with propagator (10) is the Brueckner-Sawada equation for the reaction matrix.

REDUCTION OF THE T-MATRIX EQUATION

For an interaction potential $u(\mathbf{x})$ which has a hard-core part, all the Fourier coefficients $U(\mathbf{k})$ are infinite. This difficulty can be avoided by transforming into coordinate space. It is convenient to do this with respect to only one index of T. Defining

$$t_{\mathbf{k}}(\mathbf{x}) = \frac{1}{(2\pi)^3}\int d^3k' e^{-i\mathbf{k}'\cdot\mathbf{x}} T(\mathbf{k}',\mathbf{k}),$$

Eq. (6) becomes

$$t_{\mathbf{k}}(\mathbf{x}) = u(\mathbf{x})\left[e^{-i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{(2\pi)^3} \times \int\int d^3p d^3y\, G(\mathbf{p}) e^{i\mathbf{p}\cdot(\mathbf{y}-\mathbf{x})} t_{\mathbf{k}}(\mathbf{y})\right]. \quad (11)$$

The function $t_{\mathbf{k}}(\mathbf{x})$ depends only on $x = |\mathbf{x}|$, $k = |\mathbf{k}|$ and the angle between $\mathbf{x}$ and $\mathbf{k}$. Equation (11) can be reduced into a set of integral equations in one real variable by expanding in spherical harmonics. We set

$$t_{\mathbf{k}}(\mathbf{x}) = \sum_{l=0}^{\infty} \tau_k^{(l)}(x) P_l(\hat{k}\cdot\hat{x}),$$

and use the formula

$$e^{i\mathbf{k}\cdot\mathbf{x}} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kx) P_l(\hat{k}\cdot\hat{x}),$$

where j_l is the spherical Bessel function, and the orthogonality relation between Legendre functions

$$\int d^2\hat{x}\, P_l(\hat{k}\cdot\hat{x}) P_m(\hat{x}\cdot\hat{k}') = \frac{4\pi}{2l+1} P_l(\hat{k}\cdot\hat{k}')\delta_{lm}.$$

Substitution into Eq. (11) gives

$$\tau_k^{(l)}(x) = (2l+1)(-i)^l j_l(kx) u(x) + \frac{2}{\pi}\int\int dy dp\, y^2 p^2 G(p) u(x) \times j_l(px) j_l(py) \tau_k^{(l)}(y). \quad (12)$$

The excitation spectrum is

$$\epsilon(k) = \left\{\left[\frac{k^2}{2m} + n_0 T(\tfrac{1}{2}k, \tfrac{1}{2}k) + n_0 T(\tfrac{1}{2}k, -\tfrac{1}{2}k) - n_0^2 T(0,0)\right]^2 - n_0^2 T(k,0)^2\right\}^{1/2}, \quad (13)$$

and the depletion is

$$n - n_0 = \frac{1}{2\pi^2}\int dk \left[\frac{(k^2/2m) + n_0 T(\tfrac{1}{2}k, \tfrac{1}{2}k) + n_0 T(\tfrac{1}{2}k, -\tfrac{1}{2}k) - n_0 T(0,0)}{2\{[(k^2/2m) + n_0 T(\tfrac{1}{2}k, \tfrac{1}{2}k) + n_0 T(\tfrac{1}{2}k, -\tfrac{1}{2}k) - n_0 T(0,0)]^2 - n_0^2 T(k,0)^2\}^{1/2}} - \frac{1}{2}\right]. \quad (14)$$

The formula

$$T(k',k) = 4\pi \sum_{l=0}^{\infty} i^l \int dx\, x^2 j_l(k'x) \tau_k^{(l)}(x) P_l(\hat{k}'\cdot\hat{k})$$

gives

$$T(\tfrac{1}{2}k, \tfrac{1}{2}k) + T(\tfrac{1}{2}k, -\tfrac{1}{2}k) - T(0,0) = 8\pi \sum_{l=0}^{\infty} (-1)^l \int dx\, x^2 j_{2l}(\tfrac{1}{2}kx) \tau_{k/2}^{(2l)}(x) - 4\pi \int dx\, x^2 \tau_0^{(0)}(x)$$

and

$$T(k,0) = 4\pi \int dx\, x^2 \tau_k^{(0)}(x).$$

If $G(p)$ is considered as a given function, Eq. (12) is an integral equation of Fredholm type. In vector form it can be written

$$\tau_k^{(l)} = f_k^{(l)} + K^{(l)} \tau_k^{(l)}.$$

The solution is

$$\tau_k^{(l)} = (1 - K^{(l)})^{-1} f_k^{(l)}.$$

The inverse operator of $1-K^{(l)}$ can be found numerically. The length of the calculations is greatly decreased by the fact that the kernel,

$$K^{(l)}(x,y)=\frac{2}{\pi}\int dp\, p^2G(p)u(x)j_l(px)y^2j_l(py),$$

does not depend on k. Only one inversion is needed for each value of l.

EXCITATION SPECTRUM

Numerical calculations have been carried out in the case of the hard-sphere potential, $u(x)=\infty$, $x<d$; $u(x)=0$, $x>d$; with $d=2.6$ Å; and in the case of the Lennard-Jones (L.J.) 6–8 potential

$$u(x)=(256/27)\epsilon[(\sigma/r)^8-(\sigma/r)^6],$$
$$\sigma=2.84\text{ Å},\quad \epsilon=6.34\text{°K},$$

which according to Haberlandt[8] gives best fit to the experimental data on the second virial coefficient of He^4 atoms.

The calculations were iterative in the sense that a form for $G(p)$ was assumed, $T(k',k)$ solved from Eq. (12), and the result used to find the next approximation for $G(p)$ from Eq. (10). It turned out that the procedure was very sensitive to the value of n_0 in Eq. (10). The iteration converges for $n_0/n=0.71$ (hard spheres) and 0.76 (Lennard-Jones potential). For higher or lower values of n_0 the maximum value of $G(k)$ at about 2 Å^{-1} increases or decreases, respectively, without limit. At the correct n_0 the form of $G(k)$ which is stable is found after a few cycles. In Fig. 1 the resulting energy spectra are shown. For comparison the neutron-diffraction results of Henshaw and Woods[9] are given. In the calculations the l values 0, 2, 4, 6, and 8 were included. At small x the function $j_l(x)$ is asymptotically equal to $x^l/1\times3\times\cdots\times(2l+1)$, and the higher l will give a negligible contribution below $k=3$ Å^{-1}.

The depletion given by Eq. (14) was found to be $(n-n_0)/n=1.74$ (hard spheres) and 1.32 (L.J. potential). Compared with the input values 0.29 and 0.24 there is a large discrepancy. In addition to approximation [4], this reflects the effect of the approximation made in the self-energy parts, and of the center-of-mass approximation. According to the computations the result of Eq. (14) is very sensitive to the form of $T(k',k)$. This probably explains the remarkable inconsistency in the values of $n-n_0$ found in previous papers. The microscopic approach can at the moment give no conclusive estimate of the magnitude of the depletion.

The qualitative behavior of the excitation spectrum is seen to be fairly independent of the details of the interaction. The sound velocity given by our calculation is somewhat larger (hard spheres) or somewhat smaller (L.J. potential) than the measured velocity, shown in Fig. 1. as the slope of the dashed line. This results from a similar variation of the calculated values $T(0,0)$ describing small momentum scattering.

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