Bose System of Hard Spheres*

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A generalized pseudopotential for hard-sphere interaction is obtained, which is valid for all angular-momentum states. This pseudopotential is then used in the evaluation of both the ground-state energy and the excitation spectrum for a dilute Bose system of hard spheres. The calculated ground-state energy agrees with that obtained by other authors; the excitation spectrum obtained for liquid helium resembles the phonon-roton spectrum introduced by Landau.

1. INTRODUCTION

THE problem of a quantum-mechanical system of many particles with hard-sphere interaction has been considered by many authors. In particular, Lee, Huang, and Yang[1] used a pseudopotential method and obtained many interesting results on both the equilibrium and nonequilibrium properties for the system under consideration. This method is based on the idea of replacing the hard-sphere boundary condition on the wave function by a pseudopotential to facilitate the perturbational calculation. The same idea was introduced by Fermi[2] in the scattering problem, but he limited the use of pseudopotential to the Born approximation. Huang and Yang[3] generalized the Fermi pseudopotential to include all the partial waves, but the form of their generalized pseudopotential is rather complicated. For this reason the calculation in LHY is still based on the S-wave Fermi pseudopotential. Henceforth many people[4–6] have made attempts to modify the Fermi pseudopotential for the purpose of simplifying the many-body calculations or to introduce some new pseudopotential with broader range of validity.

We report in this paper a new form of pseudopotential which is simple in form and gives, in general, exact results for two-body scattering problems or for many-body problems with the assumption of binary interaction. It is also, in our opinion, easier to handle than the pseudopotentials mentioned above. The derivation of this generalized pseudopotential forms the main body of Sec. 2. The other conclusion reached in Sec. 2 is that any well-behaved potential consisting of a hard-core part can be treated as the sum of a potential defined outside the core region and our generalized pseudopotential.

In Sec. 3 our generalized pseudopotential is applied to a system of many particles. We make use of the second quantization formalism and write down the hard-sphere Hamiltonian, which is independent of statistics. We then confine ourselves to a dilute Bose system in Sec. 4 and obtain its ground state energy, which agrees with that obtained by other authors. The excitation spectrum is discussed in Sec. 5. The interesting result is that if we stretch the validity of the present calculation and apply the result to liquid helium, we can produce the phonon-roton spectrum introduced phenomenologically by Landau[7] to explain the low-temperature properties of liquid helium II.

2. PSEUDOPOTENTIAL FOR HARD-SPHERE INTERACTION

For two particles with hard-sphere interaction, the wave function can be written, in general, as

$$\psi(\mathbf{r})=\sum_{l,m} A_{lm}\frac{U_l(r)}{r}Y_l^m(\theta,\varphi)$$

and the function $U_l(r)$ satisfies the Schrödinger equation

$$\frac{\hbar^2}{2\mu}\frac{d^2U_l(r)}{dr^2}+\left(E-\frac{l(l+1)\hbar^2}{2\mu r^2}\right)U_l(r)=0\,, \quad (2.1\text{a})$$

with the boundary condition

$$U_l(r)=0\,,\quad r\leqslant a\,, \quad (2.1\text{b})$$

where a is the diameter of the hard sphere. The slope $dU_l(r)/dr$ suffers a discontinuity at $r=a$. It is well known that such effect can be produced by including a δ-function term in the second-order differential equation. In general the following homogeneous differential equation reproduces the solution in (2.1):

$$\frac{\hbar^2}{2\mu}\frac{d^2u_l(r)}{dr^2}+\left(E-\frac{l(l+1)\hbar^2}{2\mu r^2}\right)u_l(r)=\lim_{\epsilon\to 0}\frac{\hbar^2}{2\mu}\delta(r-a)\frac{du_l(r+\epsilon)}{dr}\,, \quad (2.2)$$

where ϵ is a *positive* infinitesimal quantity. With the boundary condition $u_l(0)=0$, the general solution of

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[1] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957). Hereafter referred to as LHY.

[2] E. Fermi, Ricerca Sci. **7**, 13 (1936).

[3] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).

[4] T. T. Wu, Phys. Rev. **115**, 1390 (1959).

[5] E. Lieb, Proc. Natl. Acad. Sci. **46**, 1000 (1960).

[6] R. Abe, Progr. Theoret. Phys. (Kyoto) **19**, 699 (1958).

[7] L. Landua, J. Phys. (USSR) **11**, 91 (1947).

(2.2) is

$$u_l(r)=B_l kr j_l(kr)\,, \quad r<a \tag{2.3}$$

$$u_l(r)=B_l kr j_l(kr)+C_l kr[n_l(ka)j_l(kr)-j_l(ka)n_l(kr)]\,, \quad r>a \tag{2.4}$$

where j_l and n_l are the spherical Bessel and spherical Neumann functions, respectively, and $\hbar^2k^2/2\mu=E$. If we integrate both sides of (2.2) form $a-\epsilon$ to $a+\epsilon$ we obtain

$$du_l(r)/dr\,|_{r=a-\epsilon}=0\,. \tag{2.5}$$

From (2.3) and (2.5) we conclude that

$$u_l(r)=0 \quad \text{for} \quad r\leqslant a\,, \tag{2.6}$$

except when k satisfies the following equation

$$ka j_l'(ka)+j_l(ka)=0\,. \tag{2.7}$$

Equation (2.6) together with (2.4) gives exactly the solution of (2.1). From (2.2) we can write down the equation for the wave function $\psi(\mathbf{r})$ as

$$\frac{\hbar^2}{2\mu}\nabla^2\psi(\mathbf{r})+E\psi(\mathbf{r})=\lim_{\epsilon\to 0}\frac{\hbar^2}{2\mu a}\delta(r-a)\left(\frac{\partial}{\partial r}r\psi(\mathbf{r})\right)_{r=a+\epsilon}. \tag{2.8}$$

Therefore, for two-body scattering problems, the following pseudopotential can be used as an exact replacement for the hard-sphere boundary condition:

$$V_{\mathrm{ps}}\equiv\frac{\hbar^2}{2\mu a}\delta(r-a)\left(\frac{\partial}{\partial r}r\quad\right)_{r=a+\epsilon}, \tag{2.9}$$

so long as the energy of scattering does not satisfy (2.7).

We shall use the pseudopotential V_{ps} in the many-body calculation in the next section. In view of the fact that there is this discrete set of energies for which V_{ps} does not exactly replace the hard-sphere potential, we have to examine its effect on the calculated results. Our unperturbed many-body system is a collection of free particles, which have a continuous energy spectrum in the limit of infinite volume. So long as the discrete set does not cause any singularities in the perturbational calculation, we argue that it should have no effect on the calculation. As far as the present calculation is concerned, it can be seen from later sections that no such singularities occur. In a formal way this defect of V_{ps} can be corrected for by associating with it a projection operator, which selects out this particular set of states and replaces them by the exact hard-sphere solutions. A type of projection operator, which would project out the hard-sphere solution, has been proposed by Siegert.[8] But, in our opinion, such a formal mathematical scheme would not improve the present calculation for a dilute Bose system.

It is easy to see that an additional potential term in Eq. (2.2) would not change the form of the pseudopotential, so long as the added potential is nonsingular in the region $r\geqslant a$. Huang[9] in his treatment of a Van der Waal type potential breaks it into a pseudopotential part and an attractive part. Our present treatment gives the justification for this type of procedure.

3. MANY-BODY SYSTEM

We make use of the pseudopotential derived in last section to construct a many-body Hamiltonian with hard-sphere interaction between pair of particles. As in LHY we make an assumption of interaction through pairwise-pseudopotentials, namely, we take as the interaction term the following

$$H'=\lim_{\epsilon\to 0}\frac{\hbar^2}{2ma}\sum_{i>j}\delta(r_{ij}-a)\left(\frac{\partial}{\partial r_{ij}}r_{ij}\quad\right)_{r_{ij}=a+\epsilon}. \tag{3.1}$$

The validity of this approximation has been thoroughly discussed by Huang and Yang.[3] In addition, Wu[4] has proved that there should be no three-body pseudopotential. It is also doubtful that up to the order of accuracy of the present calculation, the higher body pseudopotentials would change any of our results obtained by using (3.1).

We recast (3.1) in the language of quantized fields, and with periodic boundary condition applied to a box of volume Ω, write down the many-body Hamiltonian

$$H=-\frac{\hbar^2}{2m}\int d^3x\psi^*(\mathbf{x})\nabla^2\psi(\mathbf{x})+\lim_{\epsilon\to 0}\frac{\hbar^2}{2ma}\int d^3x d^3x' \times\psi^*(\mathbf{x})\psi^*(\mathbf{x}')\delta(r-a)\left(\frac{\partial}{\partial r}r\psi(\mathbf{x}')\psi(\mathbf{x})\right)_{r=a+\epsilon}, \tag{3.2}$$

where ψ^* and ψ are the usual field operators for free particles and $r=|\mathbf{x}-\mathbf{x}'|$. The difference between periodic and rigid box boundary conditions has been discussed for hard-sphere interaction by Eyges.[10]

We use the annihilation operator a_k defined by

$$\psi(\mathbf{x})=\frac{1}{\sqrt{\Omega}}\sum_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}\,, \tag{3.3}$$

and write H in momentum space:

$$H=\frac{\hbar^2}{2m}\sum_{\mathbf{k}}k^2a_{\mathbf{k}}^*a_{\mathbf{k}}+\lim_{\epsilon\to 0}\frac{2\pi a\hbar^2}{m\Omega}\sum_{\mathbf{p},\mathbf{q},\mathbf{s},\mathbf{t}}\delta_{\mathbf{p}+\mathbf{q}-\mathbf{s}-\mathbf{t},0}a_{\mathbf{p}}^*a_{\mathbf{q}}^*a_{\mathbf{s}}a_{\mathbf{t}} \times\left\{\frac{\sin Qa}{Qa}+\frac{a+\epsilon}{2}\frac{\mathbf{Q}\cdot(\mathbf{t}-\mathbf{s})}{Q}\left(\frac{\cos Qa}{Qa}-\frac{\sin Qa}{(Qa)^2}\right)\right\}, \tag{3.4}$$

where

$$\mathbf{Q}\equiv-\tfrac{1}{2}\{(\mathbf{p}-\mathbf{q})-(\mathbf{t}-\mathbf{s})(1+\epsilon/a)\}\,.$$

It is to be noticed that the factor ϵ in the definition of $\mathbf{Q}$ is indispensable in getting the correct results. The Hamiltonian (3.4) is independent of statistics.

[8] A. J. F. Siegert, Phys. Rev. **116**, 1057 (1959).

[9] K. Huang, Phys. Rev. **119**, 1129 (1960).

[10] L. Eyges, Ann. Phys. (N. Y.) **2**, 101 (1957).

4. GROUND-STATE ENERGY FOR A DILUTE BOSE SYSTEM

We apply (3.4) specifically to a dilute Bose system consisting of N particles. We adopt Bogoliubov's[11] approximation in replacing the creation and annihilation operators for zero momentum particles, a_0^* and a_0, by a c number, $(N_0)^{1/2}$, where N_0 is the occupation number for the zero-momentum state. In this approximation, the Hamiltonian H in (3.4) can be rewritten as

$$H=H_p+H_t+H_r\,, \tag{4.1}$$

$$H_p=\frac{\hbar^2}{2m}\Bigg\{4\pi a\rho N[1+(1-\xi)^2] +\lim_{\epsilon\to 0}\sum_{\mathbf{k}\neq 0}\bigg[(k^2+k_0^2f(k))a_{\mathbf{k}}^*a_{\mathbf{k}}+\frac{k_0^2}{2}\frac{\sin ka}{ka}a_{\mathbf{k}}^*a_{-\mathbf{k}}^* +\frac{k_0^2}{2}\cos k(a+\epsilon)a_{\mathbf{k}}a_{-\mathbf{k}}\bigg]\Bigg\}\,, \tag{4.2}$$

$$H_t=\lim_{\epsilon\to 0}\frac{4\pi a\hbar^2}{m\Omega}(N\xi)^{1/2}\sum_{\mathbf{p},\mathbf{q},\mathbf{p}+\mathbf{q}\neq 0}\{g_+(\mathbf{p},\mathbf{q})a_{\mathbf{p}}^*a_{\mathbf{q}}^*a_{\mathbf{p}+\mathbf{q}} +g_-(\mathbf{p},\mathbf{q})a_{\mathbf{p}+\mathbf{q}}^*a_{\mathbf{p}}a_{\mathbf{q}}\}\,, \tag{4.3}$$

$$H_r=\lim_{\epsilon\to 0}\frac{2\pi a\hbar^2}{m\Omega}\sum_{\mathbf{p},\mathbf{q},\mathbf{s},\mathbf{t}\neq 0}\delta_{\mathbf{p}+\mathbf{q}-\mathbf{s}-\mathbf{t},0}\,a_{\mathbf{p}}^*a_{\mathbf{q}}^*a_{\mathbf{s}}a_{\mathbf{t}} \times\bigg\{\frac{\sin Qa}{Qa}+\frac{a+\epsilon}{2}\frac{\mathbf{Q}\cdot(\mathbf{t}-\mathbf{s})}{Q} \times\bigg(\frac{\cos Qa}{Qa}-\frac{\sin Qa}{(Qa)^2}\bigg)\bigg\}\,. \tag{4.4}$$

The symbols used in (4.2) and (4.3) are defined in the following:

$$\rho=\lim_{\substack{N\to\infty\\ \Omega\to\infty}}\frac{N}{\Omega}\,,$$

$$\xi=N_0/N\,,$$

$$k_0^2=8\pi a\rho\xi\,,$$

$$f(k)=\frac{\sin\frac{1}{2}k\epsilon}{\frac{1}{2}k\epsilon}+\frac{a+\epsilon}{2}k\bigg(\frac{\cos\frac{1}{2}k\epsilon}{\frac{1}{2}k\epsilon}-\frac{\sin\frac{1}{2}k\epsilon}{(\frac{1}{2}k\epsilon)^2}\bigg) +\frac{\sin k(a+\frac{1}{2}\epsilon)}{k(a+\frac{1}{2}\epsilon)}+\frac{a+\epsilon}{2}k\bigg(\frac{\cos k(a+\frac{1}{2}\epsilon)}{k(a+\frac{1}{2}\epsilon)} -\frac{\sin k(a+\frac{1}{2}\epsilon)}{k^2(a+\frac{1}{2}\epsilon)^2}\bigg)-1\,, \tag{4.5}$$

$$g_\pm(\mathbf{p},\mathbf{q})=\bigg\{\frac{\sin P_\pm a}{P_\pm a}+\frac{a+\epsilon}{2}\frac{\mathbf{P}_\pm\cdot(\mathbf{p}\pm\mathbf{q})}{P_\pm} \times\bigg(\frac{\cos P_\pm a}{P_\pm a}-\frac{\sin P_\pm a}{(P_\pm a)^2}\bigg)\bigg\}\,,$$

where

$$\mathbf{P}_\pm=\mathbf{p}+(\mathbf{p}\pm\mathbf{q})(\epsilon/2a)\,.$$

[11] N. N. Bogoliubov, J. Phys. (USSR) **11**, 23 (1947).

We first try to find the energy eigenvalues of the pairwise part of the Hamiltonian, H_p, by following Wu's method.[4] For the reason of completeness we have to repeat part of his treatment here. We make a Bogoliubov transformation of the form

$$b_{\mathbf{k}}=(1-\alpha_{\mathbf{k}}^2)^{-1/2}(a_{\mathbf{k}}+\alpha_{\mathbf{k}}a_{-\mathbf{k}}^*)\,,\quad b_{-\mathbf{k}}=(1-\alpha_{\mathbf{k}}^2)^{-1/2}(a_{-\mathbf{k}}+\alpha_{\mathbf{k}}a_{\mathbf{k}}^*)\,. \tag{4.6}$$

If $\alpha_{\mathbf{k}}$ is chosen to be

$$\alpha_{\mathbf{k}}=\bigg(2y_k\frac{\sin ka}{ka}\bigg)^{-1} \times\bigg[1-\bigg(1-4y_k^2\frac{\sin ka\cos k(a+\epsilon)}{ka}\bigg)^{1/2}\bigg]\,, \tag{4.7}$$

where

$$y_k=\tfrac{1}{2}k_0^2(k^2+k_0^2f(k))^{-1}\,, \tag{4.8}$$

the Hamiltonian H_p can be written as

$$H_p=E_0+\lim_{\epsilon\to 0}\sum_{\mathbf{k}\neq 0}E_{\mathrm{ex}}(k)b_{\mathbf{k}}^*b_{\mathbf{k}} +\lim_{\epsilon\to 0}\frac{\hbar^2}{2m}\sum_{\mathbf{k}\neq 0}k_0^2\bigg(\frac{\sin ka}{ka}-\cos k(a+\epsilon)\bigg)b_{\mathbf{k}}^*b_{-\mathbf{k}}^*\,, \tag{4.9}$$

where

$$E_0=\frac{\hbar^2}{2m}4\pi a\rho N[1-(1-\xi)^2]+\lim_{\epsilon\to 0}\frac{\hbar^2}{4m}\sum_{\mathbf{k}\neq 0}(k^2+k_0^2f(k)) \times\bigg[-1+\bigg(1-4y_k^2\frac{\sin ka\cos k(a+\epsilon)}{ka}\bigg)^{1/2}\bigg]\,, \tag{4.10}$$

and

$$E_{\mathrm{ex}}(k)=\frac{\hbar^2}{2m}(k^2+k_0^2f(k))\bigg(1-4y_k^2\frac{\sin ka\cos k(a+\epsilon)}{ka}\bigg)^{1/2}\,. \tag{4.11}$$

On the other hand, if the choice is

$$\bar{\alpha}_{\mathbf{k}}=(2y_k\cos k(a+\epsilon))^{-1} \times\bigg[1-\bigg(1-4y_k^2\frac{\sin ka\cos k(a+\epsilon)}{ka}\bigg)^{1/2}\bigg]\,, \tag{4.12}$$

then,

$$H_p=E_0+\lim_{\epsilon\to 0}\sum_{\mathbf{k}\neq 0}E_{\mathrm{ex}}(k)\bar{b}_{\mathbf{k}}^*\bar{b}_{\mathbf{k}} -\lim_{\epsilon\to 0}\frac{\hbar^2}{2m}\sum_{\mathbf{k}\neq 0}k_0^2\bigg(\frac{\sin ka}{ka}-\cos k(a+\epsilon)\bigg)\bar{b}_{\mathbf{k}}\bar{b}_{-\mathbf{k}}\,. \tag{4.13}$$

From either (4.9) or (4.13), the ground-state energy for H_p is given by (4.10). If we let $\Omega\to\infty$, the summation in k can be replaced by an integral and for large values of k the second term in (4.10) is asymptotically equal to the following integral:

$$-\lim_{\epsilon\to 0}\frac{\Omega k_0^4\hbar^2}{16\pi^2m}\int_0^\infty dk\frac{\sin ka\cos k(a+\epsilon)}{ka}=0\,. \tag{4.14}$$

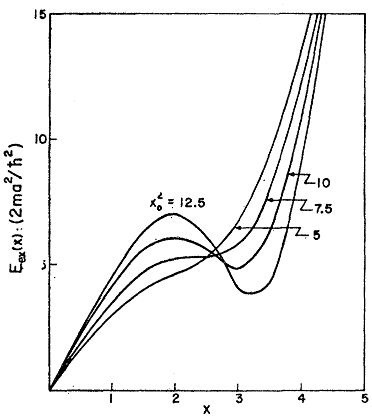

FIG. 1. Excitation energy for various values of x_0^2.

This integral is equal to zero because ϵ is positive. If we subtract from (4.10) term (4.14) with the limit taken inside the integral sign, we can interchange the integration and the limit $\epsilon\to 0$ in (4.10). Then,

$$\frac{E_0}{N}=\frac{\hbar^2}{2m}4\pi a\rho[1-(1-\xi)^2]+\frac{\hbar^2}{8m\pi^2\rho}\int_0^\infty dk\left\{k^2\left[k^2+\frac{k_0^2}{2}\left(\cos ka+\frac{\sin ka}{ka}\right)\right]\times\left[-1+\left(1-\frac{k_0^4\sin 2ka}{2ka(k^2+\frac{1}{2}k_0^2(\cos ka+\sin ka/ka))^2}\right)^{1/2}\right]+\frac{k_0^4}{2}\frac{\sin 2ka}{2ka}\right\}. \quad (4.15)$$

For $a\to 0$, the second term in (4.15) is reduced to

$$\frac{\hbar^2}{8m\pi^2\rho}\int_0^\infty dk\left\{k^2(k^2+k_0^2)\times\left[-1+\left(1-\frac{k_0^4}{(k^2+k_0^2)^2}\right)^{1/2}\right]+\frac{k_0^4}{2}\right\}. \quad (4.16)$$

This integral has been evaluated in LHY and, hence, we can just quote the result and obtain

$$\frac{E_0}{N}=\frac{2\pi\hbar^2 a\rho}{m}\left[1+\frac{128}{15\sqrt{\pi}}(a^3\rho)^{1/2}+O(a^3\rho)\right]. \quad (4.17)$$

The depletion factor ξ has been evaluated in LHY to be

$$\xi=1-\frac{8}{3\sqrt{\pi}}(a^3\rho)^{1/2}+O[(a^3\rho)], \quad (4.18)$$

which is also valid with our generalized pseudopotential. To the order of accuracy of the present calculation it is absorbed into the term $O(a^4\rho^2)$ in (4.17).

In order to carry out the next higher order term in the ground-state energy, we treat H_t by perturbation theory. For this we have to have the relevant state vectors. From (4.6), (4.7), and (4.12), we can define the right and left ground-state vectors of H_p by

$$\prod_{\mathbf{k}>0}|0_{\mathbf{k}}\rangle\equiv\prod_{\mathbf{k}>0}K_{\mathbf{k}}\exp(-\alpha_{\mathbf{k}}a_{\mathbf{k}}^*a_{-\mathbf{k}}^*)|N\rangle$$

and (4.18)

$$\prod_{\mathbf{k}>0}\langle 0_{\mathbf{k}}|\equiv\prod_{\mathbf{k}>0}\bar{K}_{\mathbf{k}}\langle N|\exp(-\bar{\alpha}_{\mathbf{k}}a_{\mathbf{k}}a_{-\mathbf{k}}),$$

where $|N\rangle$ is the N-free-particle ground-state vector, which is related to the null-particle state vector $|0\rangle$ by

$$|N\rangle\equiv\frac{1}{(N!)^{1/2}}(a_0^*)^N|0\rangle. \quad (4.19)$$

In order to have $\langle 0_{\mathbf{k}}|0_{\mathbf{k}}\rangle=1$, the product of the normalization factors in (4.18) is given by

$$K_{\mathbf{k}}\bar{K}_{\mathbf{k}}=1-\alpha_{\mathbf{k}}\bar{\alpha}_{\mathbf{k}}. \quad (4.20)$$

The state of H_p with one quasiparticle of momentum $\mathbf{k}$ excited is given by

$$|1_{\mathbf{k}}\rangle=K_{\mathbf{k}}'b_{\mathbf{k}}^*|0_{\mathbf{k}}\rangle,\quad \langle 1_{\mathbf{k}}|=\bar{K}_{\mathbf{k}}'\langle 0_{\mathbf{k}}|\bar{b}_{\mathbf{k}}, \quad (4.21)$$

where the normalization $\langle 1_{\mathbf{k}}|1_{\mathbf{k}}\rangle=1$ yields

$$K_{\mathbf{k}}'\bar{K}_{\mathbf{k}}'=(1-\alpha_{\mathbf{k}}^2)^{-1/2}(1-\bar{\alpha}_{\mathbf{k}}^2)^{-1/2}(1-\alpha_{\mathbf{k}}\bar{\alpha}_{\mathbf{k}}). \quad (4.22)$$

Now we are in a position to evaluate the non-vanishing matrix elements of H_t and write down straightforwardly the energy shift to E_0 due to H_t in second-order perturbation theory:

$$\Delta E_0=-\lim_{\epsilon\to 0}\frac{\hbar^2}{2m}\sum_{\substack{\mathbf{k}>\mathbf{k}'>\mathbf{k}''>0\\ \mathbf{k}+\mathbf{k}'+\mathbf{k}''=0}}(E_{\mathrm{ex}}(k)+E_{\mathrm{ex}}(k')+E_{\mathrm{ex}}(k'')-E_0)^{-1}256\pi^2a^2\rho\xi\Omega^{-1}(1-\alpha_{\mathbf{k}}\bar{\alpha}_{\mathbf{k}})^{-1}\times(1-\alpha_{\mathbf{k}'}\bar{\alpha}_{\mathbf{k}'})^{-1}(1-\alpha_{\mathbf{k}''}\bar{\alpha}_{\mathbf{k}''})^{-1}[g_+(\mathbf{k},\mathbf{k}')\alpha_{\mathbf{k}}\alpha_{\mathbf{k}'}-g_-(\mathbf{k},\mathbf{k}')\alpha_{\mathbf{k}''}+\mathrm{sym.}]\times[g_-(\mathbf{k},\mathbf{k}')\bar{\alpha}_{\mathbf{k}}\bar{\alpha}_{\mathbf{k}'}-g_+(\mathbf{k},\mathbf{k}')\bar{\alpha}_{\mathbf{k}''}+\mathrm{sym.}]. \quad (4.23)$$

In the limit $a\to 0$, this is reduced exactly to (4.18) in Wu's paper.[4] We refer to his careful treatment of this summation and quote his results below

$$\Delta E_0=\frac{16\hbar^2}{m}(\tfrac{4}{3}\pi-\sqrt{3})\pi a\rho N[(a^3\rho)\ln(12\pi a^3\rho)+O(a^3\rho)]. \quad (4.24)$$

In other words, we have also reproduced the logarithm term in the ground-state energy using our generalized pseudopotential. It may also be mentioned that, unlike Wu's case, the upper momentum cutoff which he has to introduce in the calculation should come out automatically because of our form of $\alpha_{\mathbf{k}}$.

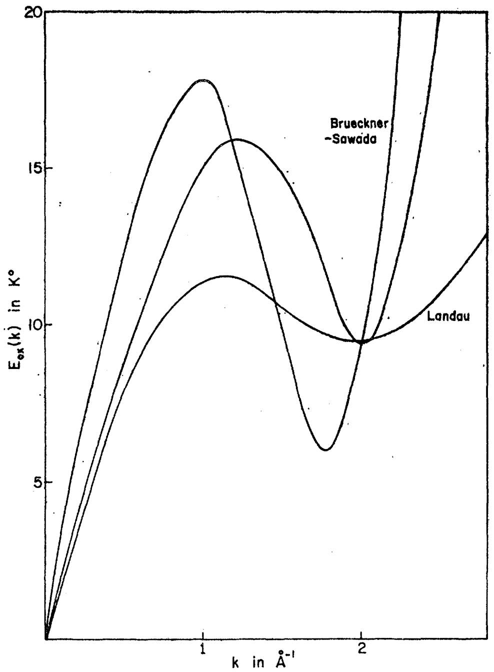

FIG. 2. Excitation energy for special choices of parameters pertinent to liquid helium II as mentioned in the text. We have used the conversion factor

$$\frac{\hbar^2}{2ma^2}=\frac{6.06}{a^2\text{ (in Å}^2)}:K^0.$$

The phenomenological curve by Landau and theoretical curve by Brueckner and Sawada are reproduced for comparison. The Landau curve is taken from Ref. 7. The analytical expression for the Brueckner-Sawada spectrum and their choice of parameters can be found in Ref. 12.

5. Phonon-Roton Spectrum

From either (4.9) or (4.13), the excitation energy of quasiparticles from diagonalizing H_p is given in (4.11). We now rewrite it in a more convenient form

$$\frac{2ma^2}{\hbar^2}E_{\text{ex}}(x)=\left[x^4+x_0^2x^2\left(\cos x+\frac{\sin x}{x}\right)+\frac{x_0^4}{4}\left(\cos x-\frac{\sin x}{x}\right)^2\right]^{1/2},\quad (5.1)$$

where

$$x\equiv ka \quad\text{and}\quad x_0\equiv k_0a.$$

We plot $E_{\text{ex}}(x)$ in Fig. 1 for different values of x_0 and it is seen that for certain values of x_0, $E_{\text{ex}}(x)$ exhibits a phonon-roton behavior proposed phenomenologically by Landau[7] to explain the superfluidity behavior of liquid He II. Similar spectrum has been obtained for hard-sphere Bose system by Brueckner and Sawada,[12] Abe,[6] and Beliaev[13] from different methods.

The present calculation for the ground-state energy or excitation spectrum is only valid for very dilute gas, for which $(a^3\rho)\ll 1$. However, we would like to stretch the validity of our calculation and apply the results to liquid He II, for which the following parameters are adopted:

$$\rho=(3.6\text{ Å})^{-3},\quad a=1.6\text{ Å}.$$

We stretch the validity of (5.1) in the following manner: We assume that the excitation spectrum valid for high values of $a^3\rho$ would have the same analytic form as in (5.1) except that the constant x_0^2 would be enhanced from its present value of $8\pi a^3\rho\xi$; the value of x_0^2 is then to be fixed by relating it to the observed sound velocity in liquid He II. According to (5.1), the sound velocity, V_s, should be related to x_0^2 by

$$V_s=\frac{\hbar}{2ma}(2x_0^2)^{1/2}.\quad (5.2)$$

The experimental value of V_s for liquid He II is 237 m/sec and this would give a value of 12 for x_0^2. A plot of E_{ex} versus k for the above-mentioned choice of parameters is given in Fig. 2, where Landau's original curve and the curve by Brueckner and Sawada are also reproduced for comparison.

Our chosen value for a is smaller than the measured scattering length for liquid He II of about 2.5 Å. This discrepancy may be accounted for by the difference of the actual soft-core potential among the helium atoms and the model hard-core potential used in the calculation.

Note added in proof. After submitting this work, we received a private communication from Marshall Luban, stating that he has taken a similar approach independently and will present his results in the near future.

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[12] K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 1128 (1957).
[13] S. T. Beliaev, Zh. Eksperim. i Teor. Fiz. **34**, 433 (1958) [translation: Soviet Phys.—JETP **7**, 299 (1958)].