part of the logarithm is πi for the part of the path just above the cut. The expression (16) is consequently.

$$\Phi(r_{nm}) = -\tfrac{1}{4}(2\pi)^3 m\hbar^{-2} r_{nm}^{-1} \int_{-2k_0}^{2k_0} (k_0^2 - \tfrac{1}{4}q^2) e^{iqr_{nm}} dq . \tag{17}$$

This integral is easy to evaluate. In fact, one sees immediately by changing the variable of integration by a factor 2 and making a partial integration that (17) is equivalent to (10) and hence to (11). The final result is thus independent of the order of integration, as one expects.

The present paper was written while I was Eastman Visiting Professor at Oxford University, and the staff of the Clarendon Laboratory join me in extending heartiest congratulations to Professor Wigner on his sixtieth birthday.

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Energy Spectrum of Elementary Excitations in Helium II*

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I. INTRODUCTION

THE elementary excitations in helium II have been the object of extensive study in the past twenty years. The phonon-roton type dispersion curve[1] was first introduced to account for superfluid properties and thermodynamic behavior of liquid helium below the λ transition line. Experiment[2] has confirmed the general dependence of excitation energy on momentum postulated on phenomenological grounds by Landau.[1] The direct observation of single excitations generated by inelastic neutron scattering yields the experimental dispersion curve shown in Fig. 1.

A quantum theory of the excitations exhibiting both the phonon and roton aspects of the phenomenological dispersion curve was first derived by Bijl[3] and later with great clarity and simplicity by Feynman.[4] Further development of the theory by Feynman and Cohen[5] led to fair agreement with the phenomenological dispersion curve. In these calculations physically plausible trial wave functions are used to compute the expectation value of the energy. A somewhat different type of calculation by Kuper,[6] based on the evaluation of phonon-phonon interaction using the Rayleigh-Schrödinger perturbation formalism, gives similar results at the one point where the numerical evaluation was carried to completion. However, Kuper regarded the agreement as partly fortuitous and pointed out several deficiencies in the calculation, some unavoidable considering the state of the theory at that time and others due to the practical limitations of a hand calculation.

The theoretical description of a single excitation developed in references 3 and 4 can be extended in a systematic manner to an arbitrary number of excitations, provided that real and virtual processes in which excitations split and coalesce and scatter are neglected.[7] In this approximation, the theory gives a "free phonon" description of the excitations with the energy formula

$$\epsilon_0(k) = \hbar^2 k^2 / 2MS(k) \tag{1}$$

plotted in Fig. 1 as the B-F curve. Here $\epsilon_0(k)$ is the energy of an excitation with momentum $\hbar\mathbf{k}$. The function $S(k)$ is the liquid structure factor derived from x-ray scattering data extrapolated to absolute zero.

We report in this paper on the evaluation of phonon-phonon interaction in the approximation of

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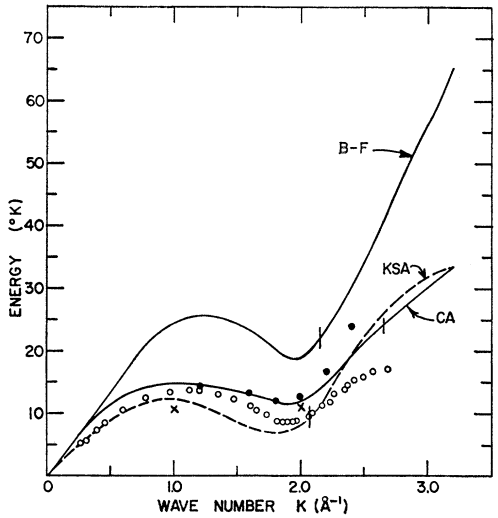

FIG. 1. The energy of elementary excitations. B-F labels the Bijl-Feynman curve calculated from Eq. (1). The curve KSA is based on the Kirkwood superposition approximation and CA is based on the convolution approximation; both were calculated using Eq. (21). The vertical lines indicate the upper limit of momentum for stable excitations. The points marked by × were calculated from the convolution approximation and the Rayleigh-Schrödinger energy formula obtained by setting $Y(k) = 0$ in the right member of Eq. (21). The open circles mark the points found experimentally by Henshaw and Woods from inelastic neutron scattering. The filled circles mark the points calculated by Feynman and Cohen using a variational calculation. Conversion of energy units is given by energy in °K = 6.061 × (energy in Å^{-2}).

the second-order Brillouin-Wigner energy formula. By using the B-W formula we avoid unphysical singularities in the computed energy shift generated by the corresponding R-S formula. Kuper[6] mentions the singularity in the long wavelength region; a second occurs when the wave number k is large enough to permit solutions of the equation

$$\epsilon_0(k) = \epsilon_0(|\mathbf{k} - \mathbf{h}|) + \epsilon_0(\mathbf{h}) \,, \quad \mathbf{h} \neq 0 \,, \tag{2}$$

implying a real phonon splitting process in the free phonon approximation.

The B-W energy formula also possesses the valuable property of giving an upper limit on the energy eigenvalue, provided of course that both second- and third-order corrections are evaluated. Our results at present are limited to the second order.

An additional, and at this time unavoidable, uncertainty is introduced by the need to use an approximation for the three-particle distribution function p (1,2,3) in evaluating matrix elements of the phonon-phonon interaction. Results are presented for the Kirkwood superposition approximation (curve KSA in Fig. 1) and a new alternative form called the convolution approximation (curve CA in Fig. 1). Both calculations agree fairly well with the experimental curve of Henshaw and Woods.[2] However, the difference between the two computed curves is large enough to encourage a determined effort to find an improved and practically useful form for p (1,2,3). In Sec. V we develop a criterion for judging the accuracy attained by any assumed form and apply it to both the KSA and CA forms.

Finally, in Sec. VI we discuss the regions of stability associated with the experimental and theoretical dispersion relations.

II. PERTURBATION PROCEDURE

We treat a system of N particles confined to a cubical box of volume Ω. The following definitions are convenient:

$\rho = N/\Omega$, mean particle density

ψ_0 is the normalized ground state solution of the Schrödinger equation with the eigenvalue E_0,

$$g(r_{12}) = \frac{(N-1)\Omega}{\rho} \int \psi_0^2 dv_{34\ldots N} \tag{3}$$

is the radial distribution function, and

$$S(k) = 1 + \rho \int [g(r) - 1] e^{i\mathbf{k}\cdot\mathbf{r}} dv$$

is the liquid structure factor. Also $U(k) = S(k) - 1$.

$$p(1,2,3) = (N-1)(N-2)\Omega \int \psi_0^2 dv_{45\ldots N}$$

is the three-particle distribution function and $\mathbf{k}$ is the discrete wave vector defined by a periodic boundary condition.

$$Q_k = \frac{1}{\sqrt{N}} \sum_m e^{i\mathbf{k}\cdot\mathbf{r}_m}$$

is the single phonon model function,

$$|\mathbf{k}\rangle = Q_{\mathbf{k}}\psi_0 / S(k)^{1/2}$$

is the normalized single phonon basis function,

$$|\mathbf{k} - \mathbf{h}, \mathbf{h}\rangle = Q_{\mathbf{k}-\mathbf{h}} Q_{\mathbf{h}} \psi_0 / [S(|\mathbf{k} - \mathbf{h}|) S(h)]^{1/2}$$

is the normalized two phonon function.

ϵ_n is the nth order B-W energy correction; explicitly for $n = 2$

$$\epsilon_2(k) = \frac{1}{2} \sum_{\mathbf{h} \neq 0} \frac{|\langle \mathbf{k}|\delta H|\mathbf{k} - \mathbf{h}, \mathbf{h}\rangle|^2}{\epsilon(k) - \epsilon_0(|\mathbf{k} - \mathbf{h}|) - \epsilon_0(h)}$$

$$\delta H = H - E_0 - \epsilon_0(k) \,.$$

The energy of an excitation is certainly smaller

than the smallest positive $\epsilon(k)$ defined by the sequence of implicit equations

$$\epsilon(k) = \epsilon_0(k) + \frac{\epsilon_2^2(k)}{\epsilon_2(k) - \epsilon_3(k)}$$

$$\epsilon(k) = \epsilon_0(k) + \frac{\epsilon_2^2(k)}{\epsilon_2(k) - \epsilon_3(k)} + \frac{(\epsilon_2\epsilon_4 - \epsilon_3^2)^2}{(\epsilon_2 - \epsilon_3)[(\epsilon_2 - \epsilon_3)(\epsilon_4 - \epsilon_5) - (\epsilon_3 - \epsilon_4)^2]} \quad (4)$$

etc.[8–10] Results based on $\epsilon_2(k)$ alone are computed from the equation

$$\epsilon(k) = \epsilon_0(k) + \epsilon_2(k) . \quad (5)$$

We surmise, comparing the curves plotted in Fig. 1, that the error introduced by neglecting ϵ_3 and higher order corrections is no greater than that associated with the approximate forms for p (1,2,3).

Unusual features of the explicit formula for $\epsilon_2(k)$ require explanation. The factor $\frac{1}{2}$ compensates for the double occurrence of the pair of wave vectors $\mathbf{k} - \mathbf{h}$, $\mathbf{h}$ in the summation (since interchanging the members of a pair does not generate a new state). The constant term in the perturbation operator δH is fixed by the requirement that $\langle \mathbf{k}|\delta H|\mathbf{k}\rangle = 0$. This in turn permits neglecting the slight failure of orthogonality in the basis functions $[\langle \mathbf{k}|1|\mathbf{k} - \mathbf{h}, \mathbf{h}\rangle \sim O(1/\sqrt{N})]$.

A useful criterion for judging the accuracy of the perturbation calculation is supplied by the statistical weight $P(k)$ of the two phonon components in the one phonon eigenfunction. This quantity is given by the formula

$$\frac{P(k)}{1 - P(k)} \cong \frac{1}{2} \sum_{\mathbf{h} \neq 0} \frac{|\langle \mathbf{k}|\delta H|\mathbf{k} - \mathbf{h}, \mathbf{h}\rangle|^2}{[\epsilon(k) - \epsilon_0(|\mathbf{k} - \mathbf{h}|) - \epsilon_0(h)]^2} \quad (6)$$

To derive Eq. (6) we observe that the perturbation formalism is simplified, if the function $|\mathbf{k} - \mathbf{h}, \mathbf{h}\rangle$ is replaced by a slightly modified function $|\mathbf{k} - \mathbf{h}, \mathbf{h}\rangle'$, orthogonal to $|\mathbf{k}\rangle$ and normalized. This substitution leaves $\epsilon_2(k)$ unchanged. The mutual nonorthogonality of the two phonon functions

$$[\langle \mathbf{k} - \mathbf{h}, \mathbf{h}|1|\mathbf{k} - \mathbf{h}', \mathbf{h}'\rangle \backsim O(1/N), \mathbf{h}' \neq \mathbf{h}]$$

is neglected.

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III. DISTRIBUTION FUNCTIONS

The two- and three-particle distributions defined in Eq. (3) are related through the sequential condition

$$\rho g(r_{12}) = \frac{1}{N - 2} \int p(1,2,3) dv_3 . \quad (7)$$

Note that Eq. (7) does not determine $p(1,2,3)$ uniquely. The general solution contains a particular solution of the inhomogeneous equation plus a solution of the homogeneous equation $\int p(1,2,3) dv_3 = 0$. Also

$$\rho \int [g(r) - 1] dv = -1 . \quad (8)$$

These relations provide a means of testing approximate forms for $p(1,2,3)$. In particular, the Kirkwood form

$$p_K(1,2,3) = \rho^2 g(r_{12}) g(r_{23}) g(r_{31}) \quad (9)$$

comes deceptively close to satisfying Eq. (7). This can be seen easily by introducing the "hole" function

$$f(r) = 1 - g(r) \quad (10)$$

and using it to separate variables in $p_K(1,2,3)$. With the help of Eq. (8), the right-hand member of Eq. (7) reduces to

$$\rho g(r_{12})[1 + \frac{\rho}{N - 2} \int f(r_{13}) f(r_{23}) dv_3] . \quad (11)$$

Thus, the error term is of order $(1/N)$, but is by no means negligible. It is just the failure of $p_K(1,2,3)$ to represent the three-particle correlations accurately, when all three particles are within the nearest-neighbor distance, that shows up in the error term.

An alternative form which satisfies Eq. (7) exactly is given by

$$\begin{aligned} p_C(1,2,3) &= p_K(1,2,3) - \rho^2[\rho \int f(r_{14}) f(r_{24}) f(r_{34}) dv_4 \\ &\quad - f(r_{12}) f(r_{23}) f(r_{31})] \\ &= \rho^2[1 - f(r_{12}) - f(r_{23}) - f(r_{31}) \\ &\quad + f(r_{12}) f(r_{23}) + f(r_{23}) f(r_{31}) + f(r_{31}) f(r_{12}) \\ &\quad - \rho \int f(r_{14}) f(r_{24}) f(r_{34}) dv_4] . \end{aligned} \quad (12)$$

We call $p_C(1,2,3)$ the convolution approximation (CA). This form suffers from the major defect that it does not vanish when two particles coincide. Nevertheless, it is useful in estimating matrix elements of non-singular operators, such as occur in the present calculation.

IV. EVALUATION OF MATRIX ELEMENTS

The procedure described in reference 7 yields

$$\int Q^*_{\mathbf{k}-\mathbf{h}} Q_{\mathbf{k}-\mathbf{h}} Q^*_{\mathbf{h}} Q_{\mathbf{h}} \psi_0^2 dv_{12\ldots N} = S(|\mathbf{k}-h|)S(h) \quad (13)$$

To compute $\langle \mathbf{k}-\mathbf{h}, \mathbf{h}|1|\mathbf{k}\rangle$ observe that

$$Q^*_{\mathbf{k}-\mathbf{h}} Q^*_{\mathbf{h}} Q_{\mathbf{k}} = N^{-3/2} \sum_{m,n,p} e^{i\{\mathbf{k}\cdot\mathbf{r}_m - (\mathbf{k}-\mathbf{h})\cdot\mathbf{r}_n - \mathbf{h}\cdot\mathbf{r}_p\}} \rightarrow N^{-1/2} \times [1 + Ne^{i\mathbf{k}\cdot\mathbf{r}_{12}} + Ne^{i\mathbf{h}\cdot\mathbf{r}_{12}} + Ne^{i(\mathbf{k}-\mathbf{h})\cdot\mathbf{r}_{12}} + N^2 e^{i\mathbf{k}\cdot\mathbf{r}_{12}} e^{i\mathbf{h}\cdot\mathbf{r}_{23}}], \quad (14)$$

the arrow signifying that equivalent terms are lumped together and numbers like $N-1$ and $N-2$ replaced by N. Consequently,

$$\langle \mathbf{k}-\mathbf{h},\mathbf{h}|1|\mathbf{k}\rangle = [NS(k)S(h)S(|\mathbf{k}-\mathbf{h}|)]^{-1/2} \times [-2 + S(k) + S(h) + S(|\mathbf{k}-\mathbf{h}|) + \frac{1}{\Omega}\int e^{i\mathbf{k}\cdot\mathbf{r}_{12}} e^{i\mathbf{h}\cdot\mathbf{r}_{23}} p(1,2,3) dv_{123}]. \quad (15)$$

The approximate forms for $p(1,2,3)$ in conjunction with Eq. (3) and repeated applications of the Fourier integral theorem now yield

$$\langle \mathbf{k}-\mathbf{h},\mathbf{h}|1|\mathbf{k}\rangle_K = [NS(k)S(h)S(|\mathbf{k}-\mathbf{h}|)]^{-1/2}[1 + U(k) + U(h) + U(|\mathbf{k}-\mathbf{h}|) + U(k)U(h) + U(k)U(|\mathbf{k}-\mathbf{h}|) + U(h)U(|\mathbf{k}-\mathbf{h}|) + \frac{1}{\rho}\left(\frac{1}{2\pi}\right)^3 \int U(k')U(|\mathbf{k}'+\mathbf{k}|)U(|\mathbf{k}'+\mathbf{h}|)d\mathbf{k}'] \quad (16)$$

$$\langle \mathbf{k}-\mathbf{h},\mathbf{h}|1|\mathbf{k}\rangle_C = [NS(k)S(h)S(|\mathbf{k}-\mathbf{h}|)]^{-1/2}[1 + U(k) + U(h) + U(|\mathbf{k}-\mathbf{h}|) + U(k)U(h) + U(k)U(|\mathbf{k}-\mathbf{h}|) + U(h)U(|\mathbf{k}-\mathbf{h}|) + U(k)U(h)U(|\mathbf{k}-\mathbf{h}|)] = N^{-1/2}[S(k)S(h)S(|\mathbf{k}-\mathbf{h}|)]^{1/2}. \quad (17)$$

Matrix elements of the phonon-phonon interaction are obtained from

$$\int Q^*_{\mathbf{k}-\mathbf{h}} Q^*_{\mathbf{h}} \psi_0 (H - E_0) Q_{\mathbf{k}} \psi_0 dv_{12\ldots N} = \frac{\hbar^2 N}{2M} \int \psi_0^2 \nabla_1 \{Q^*_{\mathbf{k}-\mathbf{h}} Q^*_{\mathbf{h}}\} \cdot \nabla_1 Q_{\mathbf{k}} dv_{12\ldots N}$$

$$= \frac{\hbar^2}{2M\sqrt{N}} [\mathbf{k}\cdot(\mathbf{k}-\mathbf{h})S(h) + \mathbf{k}\cdot\mathbf{h}S(|\mathbf{k}-\mathbf{h}|)] = \frac{\hbar^2}{2M\sqrt{N}} [k^2 + \mathbf{k}\cdot(\mathbf{k}-\mathbf{h})U(h) + \mathbf{k}\cdot\mathbf{h}U(|\mathbf{k}-\mathbf{h}|)]. \quad (18)$$

Equations (16)–(18) yield

$$\langle \mathbf{k}-\mathbf{h},\mathbf{h}|\delta H|\mathbf{k}\rangle_C = (\hbar^2/2M\sqrt{N})[S(k)S(h)S(|\mathbf{k}-\mathbf{h}|)]^{-1/2} \times [-\mathbf{k}\cdot\mathbf{h}U(h) - \mathbf{k}\cdot(\mathbf{k}-\mathbf{h})U(|\mathbf{k}-\mathbf{h}|) - k^2 U(h)U(|\mathbf{k}-\mathbf{h}|)] \quad (19)$$

$$\langle \mathbf{k}-\mathbf{h},\mathbf{h}|\delta H|\mathbf{k}\rangle_K = \langle \mathbf{k}-\mathbf{h},\mathbf{h}|\delta H|\mathbf{k}\rangle_C + \frac{\epsilon_0(k)}{[NS(k)S(h)S(|\mathbf{k}-\mathbf{h}|)]^{1/2}} \times \left[U(k)U(h)U(|\mathbf{k}-\mathbf{h}|) - \frac{1}{\rho}\left(\frac{1}{2\pi}\right)^3 \int U(k')U(|\mathbf{k}'+\mathbf{k}|)U(|\mathbf{k}'+\mathbf{h}|)d\mathbf{k}'\right] \quad (20)$$

The behavior of these matrix elements for small and large values of k and h is summarized in Table I. Both forms give $\epsilon(k)$ proportional to k in the range $k \ll \rho^{1/3}$; however, $\epsilon(k)_C$ has the same slope as $\epsilon_0(k)$, while $\epsilon(k)_K$ has a smaller slope. Feynman states without proof that $c = \hbar^{-1}(d\epsilon_0/dk)_k = 0$ is the correct velocity of normal sound in the long wavelength region; if this statement is accepted, the corresponding result $\epsilon(k)_K = c'\hbar k$ with $c' < c$ must be interpreted as an unphysical consequence of the Kirkwood form.

TABLE I. Asymptotic behavior of the interaction matrix elements.

Interaction Matrix element	$k \ll \rho^{1/3}$ $k \ll h$	$k \gg \rho^{1/3}$ $k \gg h$	$h \ll \rho^{1/3}$ $h \ll k$	$h \gg \rho^{1/3}$ $h \gg k$
CA [Eq. (19)]	$O(k^{3/2})$	$O(k)$	$O(h^{1/2})$	$O(hU(h))$
KSA [Eq. (20)]	$O(k^{1/2})$	$O(k)$	$O(h^{-1/2})$	$O(hU(h))$

To obtain numbers from Eq. (5) we convert the sum over $\mathbf{h}$ into an integral using the level density

function $2\pi\Omega h^2 dh d\mu/(2\pi)^3$ with μ defined by $l^2 = (\mathbf{k}-\mathbf{h})^2 = k^2 + h^2 - 2kh\mu$ and $d\mu = -ldl/kh$. With $(\hbar^2/2M)Y(k) = -\epsilon(k) + \epsilon_0(k)$, Eq. (5) becomes

$$Y(k) = \frac{1}{8\pi^2 k\rho}\int_0^\infty hdh\int_{|k-h|}^{k+h} ldl\,\frac{N|\langle \mathbf{l},\mathbf{h}|\delta H|\mathbf{k}\rangle|^2(2M/\hbar^2)^2}{Y(k) + h^2/S(h) + l^2/S(l) - k^2/S(k)}\,. \tag{21}$$

an implicit equation for $Y(k)$ which is solved on a machine by a program of numerical integration and iteration.

V. AN APPROXIMATION CRITERION

The relation

$$X(F) \equiv \int \psi_0 F(H - E_0)\psi_0 dv_{12\ldots N} = 0 \tag{22}$$

holds exactly for arbitrary operator F, if ψ_0 is the exact ground state eigenfunction. The formalism of the generalized normalization integral[7,11] provides a means of expressing $X(F)$ as a functional in one or more of the distribution functions $p(1,2\ldots)$. If these functions are exact, then $X(F)$ vanishes; if approximate, the function $X_a(F)$ does not vanish and, thus, provides a measure of accuracy (the subscript a denotes use of approximate forms for the distribution functions).

Following the notation and method of reference 7 we define

$$V^* = \sum_{i<j} V(r_{ij}) - \frac{\hbar^2}{8M}\sum_i \Delta_i \ln\psi_0^2$$

$$I_N(\alpha) = \int \psi_0^2 e^{\alpha V^*} dv_{12\ldots N}$$

$$\rho g(r_{12},\alpha) = \frac{(N-1)\Omega}{I_N(\alpha)}\int \psi_0^2 e^{\alpha V^*} dv_{34\ldots N} = \rho[1 - f(r_{12},\alpha)]$$

$$S(k,\alpha) = 1 + \rho\int e^{i\mathbf{k}\cdot\mathbf{r}}[g(r,\alpha) - 1]dv$$

$$U(k,\alpha) = S(k,\alpha) - 1$$

$$S(k) = S(k,0), S'(k) = \left\{\frac{dS(k,\alpha)}{d\alpha}\right\}_{\alpha=0}$$

$$p(1,2,3;\alpha) = \frac{(N-1)(N-2)\Omega}{I_N(\alpha)}\int \psi_0^2 e^{\alpha V^*} dv_{45\ldots N}$$

$$p_K(1,2,3;\alpha) = \rho^2 g(r_{12},\alpha)g(r_{23},\alpha)g(r_{31},\alpha)$$

$$p_C(1,2,3;\alpha) = p_K(1,2,3;\alpha) + \rho^2\{f(r_{12},\alpha)f(r_{23},\alpha)f(r_{31},\alpha) - \rho\left(\frac{1}{2\pi}\right)^3\int f(r_{14},\alpha)f(r_{24},\alpha) \times f(r_{34},\alpha)dv_4\} \tag{23}$$

and observe that

$$E_0 = \left\{\frac{d}{d\alpha}\ln I_N(\alpha)\right\}_{\alpha=0} = \int \psi_0^2 V^* dv_{12\ldots N}\,. \tag{24}$$

The identity

$$\psi_0(H - E_0)\psi_0 = \left\{\frac{d}{d\alpha}\frac{1}{I_N(\alpha)}\psi_0^2 e^{\alpha V^*}\right\}_{\alpha=0} - \frac{\hbar^2}{8M}\sum_i \Delta_i\psi_0^2 \tag{25}$$

yields

$$X(F) = \left\{\frac{d}{d\alpha}\frac{1}{I_N(\alpha)}\int F e^{\alpha V^*}\psi_0^2 dv_{12\ldots N}\right\}_{\alpha=0} - \frac{\hbar^2}{8M}\sum_i\int \psi_0^2\Delta_i F dv_{12\ldots N}\,. \tag{26}$$

Among the nontrivial choices for F are

$$\text{(a)}\quad Q_{\mathbf{k}}^* Q_{\mathbf{k}}$$
$$\text{(b)}\quad Q_{\mathbf{k}} Q_{\mathbf{h}}^* Q_{\mathbf{k}-\mathbf{h}}^*$$
$$\text{(c)}\quad Q_{\mathbf{k}} Q_{\mathbf{h}} Q_{\mathbf{l}} Q_{\mathbf{k}+\mathbf{h}+\mathbf{l}}^*\,. \tag{27}$$

No approximations are required to evaluate all terms occuring in $X(Q^*Q)$. Using the definitions in Eq. (23) we get

$$S'(k) = (\hbar^2 k^2/4M)[1 - S(k)] \tag{28}$$

a relation derived less directly in reference 7.

[11] F. Iwamoto and M. Yamada, Progr. Theoret. Phys. (Kyoto) **13**, 467 (1955).

To compute $X(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}})$ we use Eqs. (16) and (17) as patterns, and write

$$\left[\frac{1}{I_N(\alpha)}\int\psi_0^2 e^{\alpha V^*}Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}}dv_{12\ldots N}\right]_K = \frac{1}{\sqrt{N}}\,[1 + U(k,\alpha) + U(h,\alpha) + U(|\mathbf{k}-\mathbf{h}|,\alpha)$$
$$+ U(k,\alpha)U(h,\alpha) + U(k,\alpha)U(|\mathbf{k}-\mathbf{h}|,\alpha) + U(h,\alpha)U(|\mathbf{k}-\mathbf{h}|,\alpha)$$
$$+ \frac{1}{\rho}\left(\frac{1}{2\pi}\right)^3\int U(k',\alpha)U(|\mathbf{k}'+\mathbf{k}|,\alpha)U(|\mathbf{k}'+\mathbf{h}|,\alpha)d\mathbf{k}'] \tag{29}$$

$$\left[\frac{1}{I_N(\alpha)}\int\psi_0^2 e^{\alpha V^*}Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}}dv_{12\ldots N}\right]_C = (1/\sqrt{N})S(k,\alpha)S(h,\alpha)S(|\mathbf{k}-\mathbf{h}|,\alpha)\,. \tag{30}$$

Also

$$\sum_i \Delta_i Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}} \to -\frac{1}{\sqrt{N}}$$
$$\times [k^2Ne^{i\mathbf{k}\cdot\mathbf{r}_{12}} + h^2Ne^{i\mathbf{h}\cdot\mathbf{r}_{12}} + (\mathbf{k}-\mathbf{h})^2Ne^{i(\mathbf{k}-\mathbf{h})\cdot\mathbf{r}_{12}} + \{k^2+h^2+(\mathbf{k}-\mathbf{h})^2\}Ne^{i(\mathbf{h}\cdot\mathbf{r}_{12}+\mathbf{k}\cdot\mathbf{r}_{23})}] \tag{31}$$

The combination of Eqs. (26) and (28–31) results in

$$(8M\sqrt{N}/\hbar^2)X_K(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}}) = \{(\mathbf{k}-\mathbf{h})^2 - k^2 - h^2\}U(k)U(h) + \{k^2 - h^2 - (\mathbf{k}-\mathbf{h})^2\}U(h)U(|\mathbf{k}-\mathbf{h}|)$$
$$+ \{h^2 - k^2 - (\mathbf{k}-\mathbf{h})^2\}U(k)U(|\mathbf{k}-\mathbf{h}|) + \{k^2+h^2+(\mathbf{k}-\mathbf{h})^2\}\frac{1}{\rho}\left(\frac{1}{2\pi}\right)^3\int U(k')U(|\mathbf{k}'+\mathbf{k}|)$$
$$\times U(|\mathbf{k}'+\mathbf{h}|)d\mathbf{k}' - \frac{2}{\rho}\left(\frac{1}{2\pi}\right)^3\int\{k'^2 + (\mathbf{k}'+\mathbf{k})^2 + (\mathbf{k}'+\mathbf{h})^2\}U(k')U(|\mathbf{k}'+\mathbf{k}|)U(|\mathbf{k}'+\mathbf{h}|)d\mathbf{k}' \tag{32}$$

$$(8M\sqrt{N}/\hbar^2)X_C(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}}) = \{(\mathbf{k}-\mathbf{h})^2 - k^2 - h^2\}U(k)U(h) + \{k^2 - h^2 - (\mathbf{k}-\mathbf{h})^2\}U(h)U(|\mathbf{k}-\mathbf{h}|)$$
$$+ \{h^2 - k^2 - (\mathbf{k}-\mathbf{h})^2\}U(k)U(|\mathbf{k}-\mathbf{h}|) - \{k^2+h^2+(\mathbf{k}-\mathbf{h})^2\}U(k)U(h)U(|\mathbf{k}-\mathbf{h}|)\,. \tag{33}$$

Note that these functions are symmetrical in the three variables $\mathbf{k}$, $\mathbf{h}$, $\mathbf{k}-\mathbf{h}$, even though the symmetry is not obvious in the integrand of the integrals occuring in Eq. (32).

Both functions approach zero rapidly as k increases beyond 2Å^{-1}; otherwise they behave rather differently. Consider first $k = 0$: $X_C(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}})$ vanishes for all values of $\mathbf{h}$, while $X_K(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}})$ is definitely nonvanishing, except at $h = \infty$ and possibly one or two finite points. This difference may be correlated with the different behaviors of the corresponding interaction matrix elements for small values of k as exhibited in Table I and discussed in the text following Table I.

A second interesting comparison results from computing the integral of X over $\mathbf{h}$ space:

$$\frac{8M\sqrt{N}}{\hbar^2}\int X_K(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}})d\mathbf{h} = 2\int\mathbf{h}\cdot(\mathbf{k}-\mathbf{h})U(h)U(|\mathbf{k}-\mathbf{h}|)d\mathbf{h}$$
$$-\frac{2}{\rho}\left(\frac{1}{2\pi}\right)^3\int[\mathbf{k}'\cdot(\mathbf{k}'+\mathbf{k}) + (2\mathbf{k}'+\mathbf{k})\cdot(\mathbf{k}'+\mathbf{h})]U(|\mathbf{k}'+\mathbf{k}|)U(|\mathbf{k}'+\mathbf{h}|)U(k')d\mathbf{k}'d\mathbf{h}\,. \tag{34}$$

One integral vanishes, because the integrand is an odd function of $\mathbf{k}'+\mathbf{h}$; the remaining integrals cancel in virtue of the relation

$$\frac{1}{\rho}\left(\frac{1}{2\pi}\right)^3\int U(k)d\mathbf{k} = -1\,, \tag{35}$$

a consequence of Eq. (8) and $g(o) = 0$. Thus,

$$\int X_K(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}})d\mathbf{h} = 0\,. \tag{36}$$

The corresponding integral of X_C does not appear to vanish except possibly at isolated points.

VI. STABILITY OF ELEMENTARY EXCITATIONS

An elementary excitation may split into two or more if energy and momentum are conserved in the process. The necessary conditions are

(a) $$\epsilon(k) = \sum_{i=1}^{m} \epsilon(k_i)$$

(b) straight line segments of lengths k, k_1, k_2, . . . k_m can form the sides of a closed polygon. The process will occur unless the transition matrix element vanishes.

For any given or assumed dispersion curve one can determine the range in which conditions a and b hold by a graphical analysis. The dispersion curve is traced onto transparent sheets which are then superimposed in an appropriate manner to select out sets k, k_1, k_2, . . . k_n consistent with condition a. The possibility that b also holds is then examined.

Feynman[4] observed that the necessary conditions are satisfied in any region where the derivative $d\epsilon/dk$ is greater than the initial slope (at $k = 0$). In fact, the conditions are met in any region where the absolute value of the derivative exceeds the initial slope. The characteristic process is then decay into one relatively large quantum and one or more small quanta. Feynman's criterion determines the vertical lines on the BF and KSA curves of Fig. 1 marking the upper limit on the region of stability.

The experimental curve represents stable excitations over the entire range provided that any extension of the curve beyond $k = 2.68$Å^{-1} has positive slope.[12-14] However, it is clear that a continuation with even a small positive slope makes possible a decay process in which splitting into two excitations with nearly equal energies occurs. A decay process of this type determines the vertical line on the CA curve of Fig. 1 marking the upper limit on the region of stability.

Suppose elementary excitations are possible in the liquid beyond $k = 2.68$Å^{-1} and also that the extended dispersion curve is a continuous function with continuous first derivative. By graphical analysis one can prove the following statements (cf. Fig. 2):

(a) excitations with energies rising above the dashed line U meet the necessary conditions for instability.

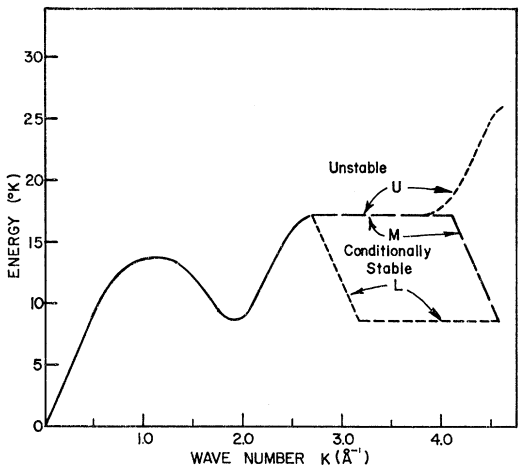

FIG. 2. Stability of elementary excitations. The solid curve is that found experimentally by Henshaw and Woods from inelastic neutron scattering. Excitations with energies above the line U will be unstable; whereas if their energies lie in the region enclosed by the parallelgram, they will be conditionally stable. For discussion see Sec. VI.

(b) excitations with energies falling below the dashed line L cause instability in the range below 2.68Å^{-1}.

(c) suppose the following two conditions are met: (1) the extended dispersion curve lies higher than the minimum roton energy (near 2Å^{-1}), and (2) every section of the extended dispersion curve satisfying $L < \epsilon < M$ also satisfies $|d\epsilon/dk| < |d\epsilon/dk|_{k=0}$. Then every section satisfying $L < \epsilon < M$ represents excitations which are stable against splitting in any way whatsoever. Also excitations on the experimentally determined dispersion curve are stable against splitting in any way whatsoever.

VII. DISCUSSION

The solutions of Eq. (21) displayed graphically in Fig. 1 were found by an iteration process on an IBM 704 computer. The Rayleigh-Schrödinger second-order energy was evaluated at $k = 1.0$Å^{-1} and 2.0Å^{-1}, using the convolution approximation by setting $Y(k) = 0$ in the right-hand member of Eq. (21). These results appear in Fig. 1. For the liquid structure factor, we used the experimental curve determined by Goldstein and Reekie[15] at 2.06°K with modifications introduced by Feynman and Cohen to insure correct behavior at absolute zero. These modifications are (a) linear extrapolation to the origin at $k = 0$, (b) multiplication throughout by a factor 0.97 to satisfy $g(0) = 0$, and (c) smooth extrapolation from 6.0 to 7.2Å^{-1} and for $k > 7.2$Å^{-1},

[12] Pitaevskiĭ has investigated the properties of the elementary excitation spectrum near the disintegration threshold by studying the appropriate Green's functions.[13] In particular, he has discussed[14] the type of threshold which seems to apply to the experimentally determined spectrum at normal vapor pressure.[2]

[13] L. P. Pitaevskiĭ, Soviet Phys.—JETP 9, 830 (1959).

[14] L. P. Pitaevskiĭ, Soviet Phys.—JETP 12, 155 (1961).

[15] L. Goldstein and J. Reekie, Phys. Rev. 98, 857 (1955).

$S(k) = 1$. Modification (a) results in a slope for the dispersion curves $\epsilon_a(k)$ and $\epsilon(k)_C$ at the origin corresponding to a sound velocity of 366 m/sec, about 50% greater than the directly measured sound velocity (238 m/sec). We have not succeeded in resolving this discrepancy.[16]

The integral in Eq. (21) was evaluated by Simpson's rule with grids chosen to limit the relative error to less than 2 or 3% in the region $k \geqq 0.6\text{Å}^{-1}$. In the region $k < 0.6\text{Å}^{-1}$, we estimate the absolute error in $Y(k)$ from this source to be no greater than 0.01Å^{-1}. Additional uncertainties in the calculation arise from two principal sources: (1) experimental error in the liquid structure factor (estimated by Goldstein and Reekie at 5 to 7% in the region $k > 0.9\text{Å}^{-1}$) and (2) error due to use of the approximate forms for $p(1,2,3)$. To study (2), we evaluated the functions $X_C(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}})$ and $X_K(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}})$ at each grid point used in computing the integral in Eq. (21). The results reveal that $|X_C| \ll |X_K|$ in the range $k \leqq 0.6\text{Å}^{-1}$ for a wide range of values of $\mathbf{h}$ and $\mathbf{k} - \mathbf{h}$; thus, supporting the inference already stated that the convolution form yields a more accurate evaluation of the interaction matrix element for small values of k. Beyond $k = 0.6\text{Å}^{-1}$, X_C and X_K take on roughly the same range of values so we have no basis for preferring one approximate form to the other.

The quantity $P(k)$ defined by Eq. (6) was evaluated at $k = 1.0$ and 2.0Å^{-1}, using the convolution approximation, with the following results:

$$P(1.0) = 0.20, \quad P(2.0) = 0.12$$

showing that the dominant component in the one-phonon state is just the single "free" phonon basis function.

We conclude with a brief statement on the problem of determining an improved form for the three-particle distribution function. Any modified improved form should be invariant under permutations, rotations, displacements, and reflections of the coordinates. It should be positive valued when no two particles coincide and vanish when any pair (or all three) coincide. When particle 3 is far from the other two, p_a should reduce to $\rho^2 g(r_{12})$. These general conditions are supplemented by the requirement of Eq. (7) and a general statement of the X criterion

$$|X_\alpha(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}})| \ll |X_K(Q_{\mathbf{k}}Q^*_{\mathbf{k}-\mathbf{h}}Q^*_{\mathbf{h}})|_{\text{average}}. \quad (37)$$

The power of this criterion resides in the fact that it is required to hold for all values of k, h, and cos $(\mathbf{k},\mathbf{h})$. Thus, it is in fact a triply infinite set of conditions. In an obscure but real sense, the validity of Eq. (37) implies that $p_a(1,2,3)$ can be computed from a trial function which closely approximates the ground state eigenfunction.

VIII. SUMMARY

The contribution of phonon-phonon interaction to the energy of elementary excitations in liquid He^4 is evaluated in the approximation of the Brillouin-Wigner second order energy. The three-particle distribution function $p(1,2,3)$ occurring in the interaction matrix elements is approximated by the Kirkwood superposition form and also by the "convolution" form.

A general criterion is developed to test the accuracy of possible approximations for $p(1,2,3)$. The criterion has the form of a functional X in $p(1,2,3)$ which vanishes if $p(1,2,3)$ is generated by the correct ground state solution of the Schrödinger equation. If an approximate form is used the corresponding functional X_a does not vanish and thus provides a measure of accuracy. The power of this criterion resides in the fact that X_a is a function of three variables, the magnitudes of two wave vectors and the cosine of the angle between them.

The computed dispersion curves are compared with the experimental curve constructed by Henshaw and Woods from the inelastic single scattering of slow neutrons in liquid helium.

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[16] We are indebted to Dr. Michael Cohen for verifying this discrepancy (private communication). *Added in proof:* Miller, Pines, and Nozieres discuss a possible remedy (preprint).