Polarization Potentials and Elementary Excitations in He II at Low Temperatures*

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(Received June 14, 1976)

The density fluctuation excitation spectrum of He II is calculated using a generalized polarization potential approach and shown to yield a phonon–roton spectrum for wave vectors less than $2.1 \, \text{Å}^{-1}$ in excellent quantitative agreement with that observed in neutron scattering experiments for pressures ranging from SVP to ~25 bar. The model provides a simple physical explanation for the increase in maxon energy and decrease in roton energy with increasing pressure, and a quantitative account of the pressure variation of the single-phonon energy and probability amplitude in the vicinity of the roton minimum $(1.8 \leq q \leq 2.1 \, \text{Å}^{-1})$.

1. INTRODUCTION

Elementary excitations observed in the density fluctuation excitation spectrum of quantum liquids at frequencies ω_q and wave vectors $\mathbf{q}$ such that one is in the collisionless regime $(\omega_q \tau \gg 1$, where τ is a characteristic relaxation time) must have their origin in the averaged self-consistent field $\langle \rho(q, \omega) \rangle$ of all the particles acting in concert. In superfluid He II it was believed that such a field owes its presence to the condensate, until experiments by Cowley and Woods[1,‡] showed that well-defined excitation modes with wave vectors in the range $0.2 < q \lesssim 0.6 \, \text{Å}^{-1}$ persist with virtually unchanged energies at temperatures well above the λ point. It was therefore suggested by Pines[5] that the restoring force for such modes comes instead from polarization effects produced by strong short-range correlations and that these modes represent the analog, for a neutral system, of the plasma

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oscillations characteristic of charged particle systems. The existence of such modes had already been proposed, on the basis of physical arguments and an RPA calculation, some years earlier, by Pines and Bohm[3]; in subsequent work it was argued that a description of particle interaction in terms of phenomenological polarization potentials,[4] analogous to those employed by Leggett[5] in his formulation of the Landau–Fermi liquid theory, would provide a useful starting point for a calculation of the He II excitation spectrum. In this communication we show that this is indeed the case: we obtain excellent agreement between theory and experiment at SVP by introducing only two q-dependent potentials (one scalar, one vector), whose basic form is derived from simple physical arguments and a fit to selected points on the excitation spectrum. We propose a simple model, with no adjustable parameters, for the way in which these potentials vary with pressure, and show that it provides a good account of the pressure dependence of the excitation spectrum.

   The restoring force responsible for the excitation spectrum derives, in large part, from a scalar polarization potential,[2] which takes the form

$$\phi_{\text{pol}}(q\omega) = f_q^s \langle \rho(q\omega) \rangle \tag{1}$$

Here $\langle \rho(q\omega) \rangle$ is the density fluctuation induced by an external scalar probe, and ϕ_{pol} couples directly to the density fluctuations in the system. ϕ_{pol} does not, however, describe an important physical effect arising in a strongly interacting system; a given particle, as it moves through the system, will drag along other particles, so that its effective mass may be considerably increased over its free-particle value m_0. This latter effect may be taken into account by introducing a vector polarization potential,

$$\mathbf{A}_{\text{pol}}(q\omega) = f_q^v \langle \mathbf{J}(q, \omega) \tag{2}$$

which couples to the particle current density; here $\langle \mathbf{J}(q\omega) \rangle$ is the current density fluctuation induced by the external scalar probe. The density–density response function then takes the form

$$\chi(q, \omega) = \frac{\chi_{\text{sc}}(q, \omega)}{1 - [f_q^s + (\omega^2/q^2)f_q^v]\chi_{\text{sc}}(q, \omega)} \tag{3}$$

where χ_{sc} is the response of the density fluctuations to the external field plus the induced scalar and vector potentials, (1) and (2). One thus obtains a momentum-dependent effective mass for the quasiparticles in the system, $m_q^* = m_0 + N f_q^v$, while application of the f-sum rule leads to the asymptotic result, $\lim_{q \to \infty} \chi_{\text{sc}}(q\omega) = N q^2 / m_q^* \omega^2$, where N is the system density.

   The expression (3) may be used to calculate the density fluctuation excitation spectrum of any strongly interacting neutral system; in the case of

liquid ^{3}He and ^{4}He, one expects that the polarization potentials at compara-
ble densities will be quite similar, since in the strong-coupling limit interac-
tion effects frequently prove more important than effects of statistics. For
^{3}He, in the limit of long wavelengths and low temperatures, the theory
reduces to the usual Landau–Fermi liquid theory; it provides a natural
extension of that theory to shorter wavelengths and higher temperatures[4,6,†]
and forms the basis of a theoretical account[7] of the excitation spectrum of
^{3}He which is in good agreement with both the zero-sound mode[8] and single
pair excitation spectrum recently observed by inelastic neutron scattering.[9]
It provides as well a basis for calculating the density fluctuation excitation
spectrum of both normal and superfluid ^{4}He and of ^{3}He–^{4}He mixtures.

For He II, the screened density response function $\chi_{sc}(q\omega)$ takes the
form[4]

$$\chi_{sc}(q\omega) = \frac{\alpha_q Nq^2/m_q^*}{\omega^2 - \varepsilon_q^2} + \chi_m(q, \omega) \tag{4}$$

as long as the temperature is sufficiently low that the contribution coming
from thermally excited quasiparticles can be neglected ($T \lesssim 1$ K). The first
term on the rhs of (4) is the contribution from the excitation of single
quasiparticles of mass m_q^*, energy $q^2/2m_q^*$, from the condensate; the second
describes the excitation of two or more quasiparticles from the condensate.
As long as the frequencies of interest are low compared to the average
multiparticle energy $\bar{\omega}_q$ (typically 40 K for $q \gtrsim 1$ Å^{-1}), we may approximate
$\chi_m(q\omega)$ by its static limit, $\chi_m(q, \omega) \approx \chi_m(q, 0) = -N\mathscr{A}_q$. The renormalization
constant α_q provides a measure of the relative importance of the contribu-
tions made by the single and multiquasiparticle excitations to χ_{sc}. The
dispersion relation for the density fluctuation excitation spectrum of liquid
He II is obtained from the poles of $\chi(q, \omega)$ and is

$$1 = \left(f_q^s + \frac{\omega_q^2}{q^2} f_q^v \right) \chi_{sc}(q, \omega_q) \tag{5}$$

Comparison of (4) and (5) shows that the excitation energy ω_q depends, in
general, on the four independent parameters f_q^s, f_q^v, α_q, and $\mathscr{A}_q$. With the aid
of the neutron scattering results of Cowley and Woods[1] at SVP, a simple
physical model for $f_s(r)$, the spatial Fourier transform of f_q^s, and sum rule
arguments, we have determined the above parameters as a function of
density and have used these to calculate the static and dynamic form factors
in He II as a function of pressure. Our results are summarized and compared
with experiment in Figs. 1–5; we comment briefly on them here.

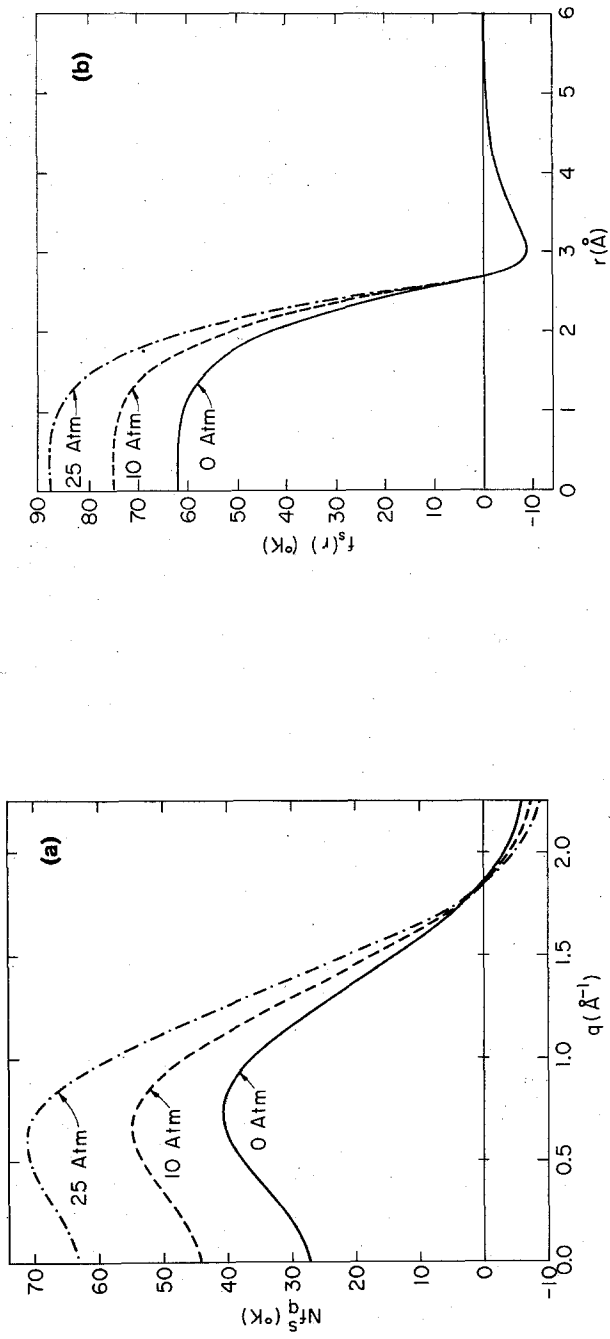†For a preliminary account of the work in Ref. 6a, see Ref. 6b.

Fig. 1. Polarization potentials and parameters for different pressures.
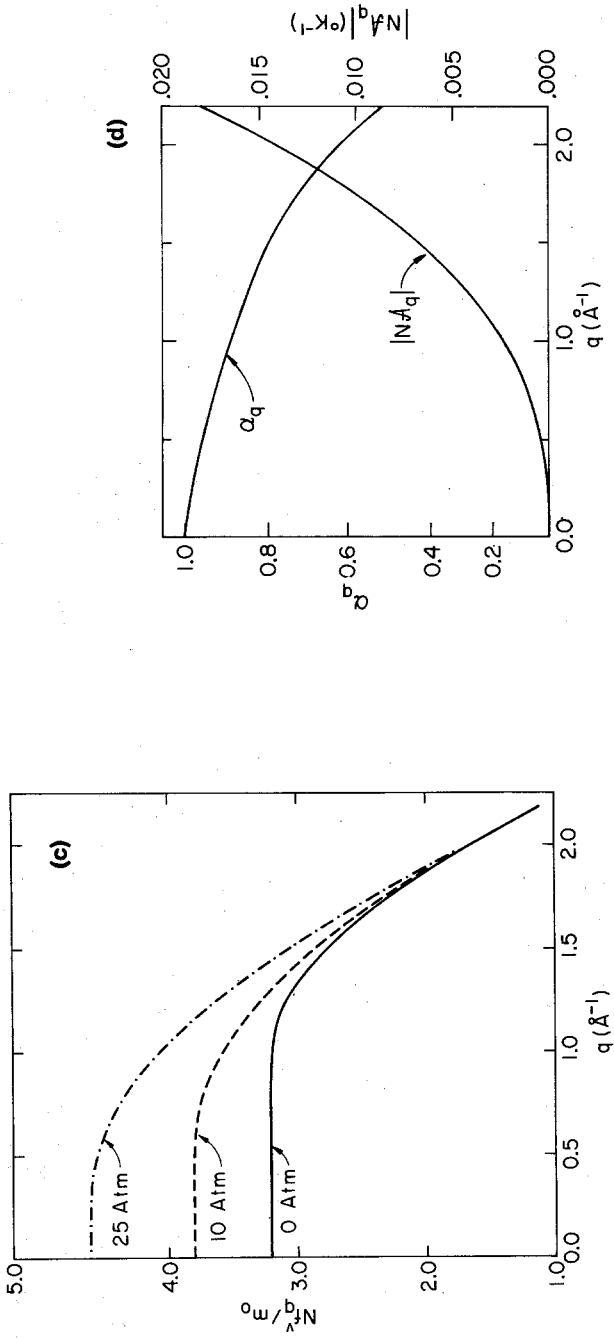
Fig. 1. Continued.

2. SCALAR POLARIZATION POTENTIAL

The scalar polarization potential f_q^s is shown as a function of pressure in Fig. 1a. The long-wavelength-limit sum-rule arguments show that

$$\lim_{q \to 0} f_q^s = m_0 s^2 / N \qquad (6)$$

where s is the isothermal sound velocity. At intermediate wave vectors and SVP, f_q^s may be determined to a good degree of approximation from the static response function $\chi(q, 0)$ measured by Cowley and Woods, by using the relation

$$-\frac{1}{\chi(q, 0)} = f_q^s + \frac{\varepsilon_q}{2N\alpha_q - N\varepsilon_q \mathscr{A}_q} \qquad (7)$$

since the second term on the rhs of (7) turns out to be negligible compared to the first as long as $q \lesssim 1.5 \text{ Å}^{-1}$. For larger wave vectors $(1.5 \lesssim q \lesssim 2.1 \text{ Å}^{-1}) f_q^s$ must be obtained self-consistently with due account taken of the other parameters, α_q, $\mathscr{A}_q$, and ε_q.

The f_q^s may be given a simple physical interpretation, as the Fourier transform of an effective interaction $f_s(r)$ between He atoms, according to

$$f_q^s = (4\pi/V) \int_0^\infty dr f_s(r) r^2 (\sin qr)/qr \qquad (8)$$

The major way in which $f_s(r)$ departs from the bare interaction potential $V(r)$ (measured in atom–atom scattering experiments) is at short distances, where the strong short-range atomic correlations present in the liquid act to reduce the hard repulsive core found experimentally to an effective soft-core interaction. We have used this result to construct a detailed model for the behavior of $f_s(r)$. We take into account the short-range correlations by adopting a simple parametrized form for the repulsive part of the effective potential, which is taken to extend to $r \sim 2.68 \text{ Å}^{-1}$; an attractive potential which is essentially that found in the atomic scattering experiments of Bennewitz et al.[10] is assumed to apply for $2.68 \lesssim r \lesssim 6 \text{ Å}^{-1}$, and the van der Waals interaction calculated by Davison[11] is assumed to describe $f_s(r)$ for $r \gtrsim 6 \text{ Å}$. The density dependence of $f_s(r)$ is obtained by assuming that, as the pressure varies, only the short-range behavior $(r \lesssim 2.68 \text{ Å}^{-1})$ of $f_s(r)$ is altered [since in our model the liquid correlations do not appreciably influence $f_s(r)$ at larger distances]; by assuming further that the shape of the soft-core repulsion is comparatively little affected by pressure, $f_s(r)$ is uniquely determined by the variation of isothermal sound velocity with

density, with the results depicted in Fig. 1b.

3. f_q^v, α_q, AND $\mathscr{A}_q$

In the limit of long wavelengths, the vector polarization potential parameter takes the form

$$\lim_{q \to 0} N f_q^v = N f_0^v = m_0^* - m_0 \qquad (9)$$

where m_0^* is the "$q = 0$" effective mass of the ^{4}He quasiparticles, a quantity not subject to direct experimental measurement. If, however, we assume that the physical effects responsible for f_0^v (strong short-range correlations and backflow) depend only weakly on temperature (and hence on statistics), we can infer m_0^* for ^{4}He by extrapolating to ^{4}He densities the known values of m_0^* for ^{3}He; in this way we obtain $N f_0^v = 3.2$ for ^{4}He at SVP, with the corresponding larger values at higher pressures shown in Fig. 1c.

Using sum rule arguments and current conservation,[12] it is straightforward to show that the long-wavelength behavior of α_q and $\mathscr{A}_q$ is given by

$$\lim_{q \to 0} \alpha_q = 1 - \alpha_2 q^2, \qquad \lim_{q \to 0} \mathscr{A}_q = -\mathscr{A}_4 q^4$$

where the quantities α_2 and $\mathscr{A}_4$ can be determined in this limit from the experimental known multiparticle contributions to the f-sum rule and static compressibility.

Once f_q^s has been determined by the procedure described above, at SVP there are only three parameters which need to be determined from three experimental quantities [$\omega_q, \chi(q, 0)$, and Z_q, the strength of the single-phonon excitation spectrum]. The SVP curves shown in Figs. 1c and 1d are determined by fitting to experiment at $q \sim 1.85^{-1}$ (where $f_q^s \sim 0$) and then extrapolating smoothly to longer and shorter wavelengths.

At higher pressures, there exist insufficient experimental data to determine α_q, $\mathscr{A}_q$, and f_q^v in this fashion; however, neutron scattering experiments suggest that the multiphonon spectrum varies only weakly with pressure.[13] We therefore make a virtue out of necessity by assuming that α_q and $\mathscr{A}_q$ vary weakly with density between SVP and 25 atm. Moreover, experiment[14] shows that Z_q and ω_q are essentially independent of pressure in the region of $q \sim 1.85$ Å^{-1}, so that one may fit the data by assuming that m_q^* and α_q are likewise independent of pressure at this wave vector. The remaining portion of the f_q^v curve is then found by extrapolating to the appropriate f_0^v limit.

We note that the multiparticle excitations begin to make an important contribution to χ_{sc} for $q \gtrsim 1$ Å^{-1}; put another way, the renormalization effects described by α_q become appreciable for such intermediate wave

vectors. For wave vectors greatly in excess of 2 Å^{-1}, multiparticle excitations may be expected to provide an increasingly important contribution to χ_{sc}; moreover, it would seem important that one take their frequency dependence into account. Since experiment provides comparatively little in the way of guidance as to how to carry out such a treatment, we have confined our attention to that portion of the excitation spectrum with wave vectors less than, say, 2.1 Å^{-1}. We further note that a smooth extrapolation of the curves in Fig. 1c suggests that the mass polarization cloud responsible for m_q^* ceases to produce appreciable changes in particle properties for $q \gtrsim 2.6\text{ Å}^{-1}$, a not unreasonable result, since one expects that at sufficiently short wavelengths the excitations in ^{4}He will behave like free particles.[15] However, mass polarization effects are still important for $q \simeq 2\text{ Å}^{-1}$.

4. ELEMENTARY EXCITATION SPECTRUM: THEORY AND EXPERIMENT

Neutron scattering experiments measure the dynamic form factor $S(q, \omega)$ of ^{4}He, which may be written as[15]

$$S(q\omega) = NZ_q\delta(\omega - \omega_q) + S^m(q\omega)$$

where Z_q is the strength of the single-phonon mode (the well-known phonon–roton spectrum) and $S^m(q\omega)$ is the contribution from the multiphonon branch of the excitation spectrum. Z_q and ω_q have been determined experimentally at SVP by Cowley and Woods[1] for $q < 3.3\text{ Å}$, while at higher pressures attention has been focused expecially on rotons and on maxons (those excitations in the vicinity of $q \sim 1\text{ Å}^{-1}$ that correspond to a local maximum in the ω_q spectrum). We have calculated ω_q and Z_q as a function of pressure, by substituting the polarization parameters shown in Fig. 1 into (5), and the analogous expression for Z_q,

$$Z_q = \frac{q^2\alpha_q}{\omega_q[m_q^*(1 - (f_q^s + \omega_q^2 f_q^v/q^2)N\mathscr{A}_q)^2 - Nf_q^v\alpha_q]}$$

The results are shown in Figs. 2 and 3, where they are compared with the experimental results of Cowley and Woods[1] at SVP and those of Henshaw and Woods[16] at 24 atm; the agreement between theory and experiment at SVP demonstrates the consistency of the various interpolative procedures we have follwed, while the pressure dependence of ω_q and Z_q provides a more stringent test of the theory presented here, since no free parameters have been introduced in our determination of the density dependence of the polarization potentials. In Fig. 4, we compare our results for the pressure
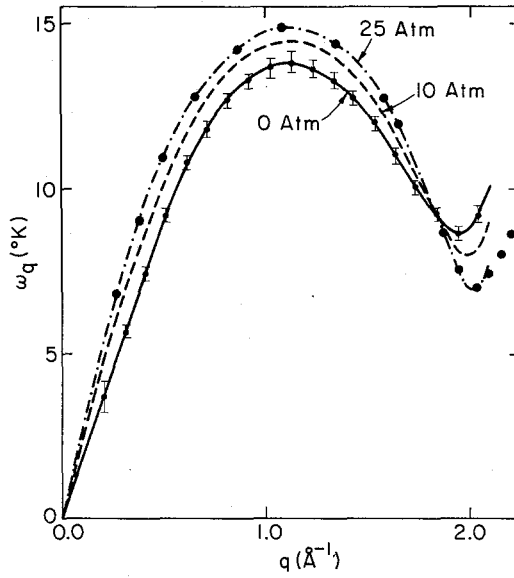
Fig. 2. The single-phonon excitation spectrum at three pressures. The experimental points at SVP are taken from Cowley and Woods,[1] while those at 25.3 atm are due to Henshaw and Woods.[12]
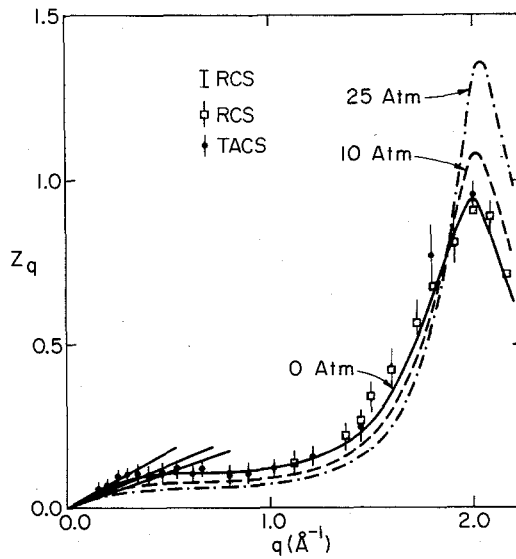

Fig. 3. The single-phonon probability amplitude Z_q at three pressures. The experimental points at SVP are due to Cowley and Woods.[1]
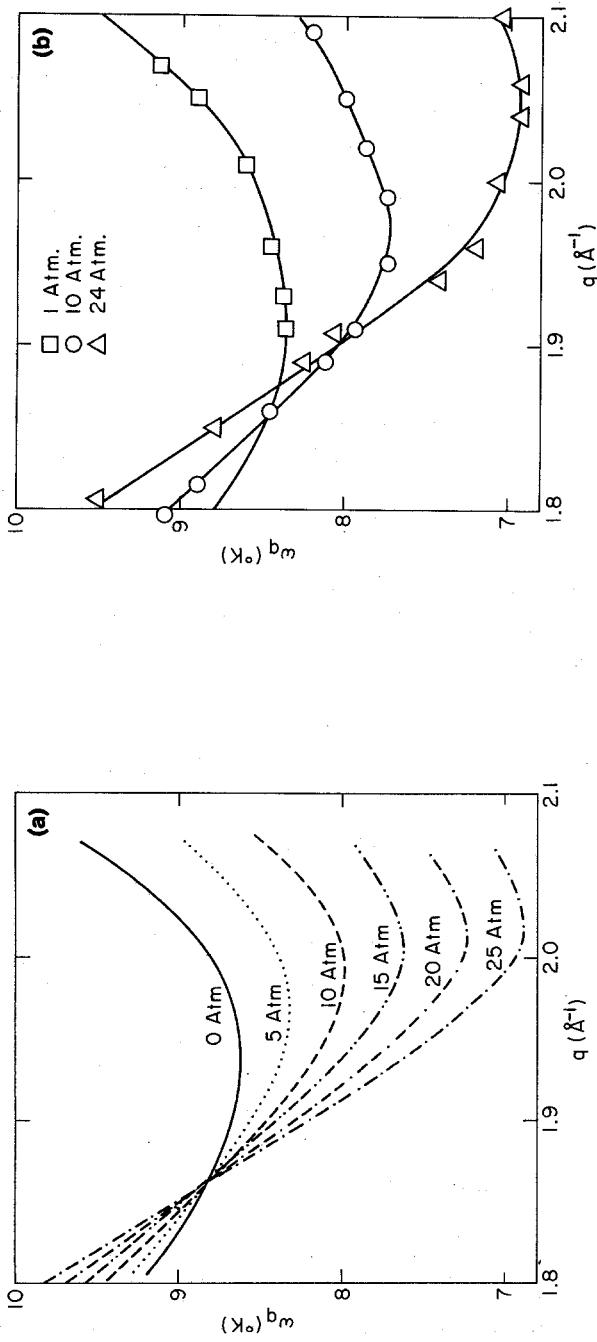
Fig. 4. Comparison of theory (a, c) with the experiments of Dietrich *et al.*[14] (b, d) for ω_q and Z_q at three pressures have been normalized by fitting to the peak value ($Z_q = 0.93 \pm 0.02$) found at SVP by Cowley and Woods.
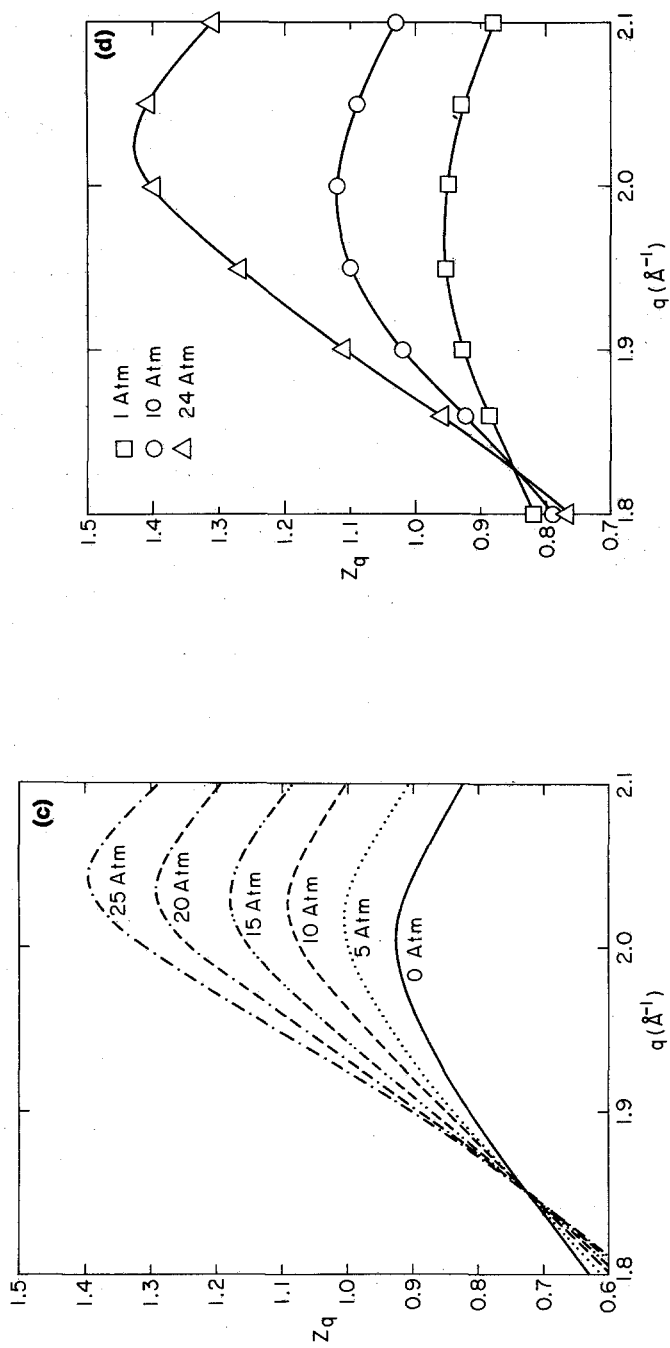
Fig. 4. Continued.

dependence of ω_q and Z_q in the region $1.8 \lesssim q \lesssim 2.1$ Å^{-1} with the experimental values of Dietrich et al.,[14] while in Fig. 5 our theoretical results for the pressure dependence of the roton and maxon energies are compared with the experimental results of Dietrich et al.[14] and Graf et al.[13]; the agreement is again seen to be good. We further note that at 20 atm in the maxon region Z_q drops to about 50% of its SVP value, in agreement with the qualitative measurements of Woods et al.[17]

Both the increase of the maxon energy and the decrease of the roton energy with pressure may be directly attributed to the increasing "hardness" of the repulsive soft-core potential $f_s(r)$ displayed in Fig. 1b; the shape of ω_q and Z_q near the roton minimum likewise provides a sensitive measure of the variation with pressure of the shape and strength of the repulsive part of $f_s(r)$.

We have calculated as well the influence of pressure on the long-wavelength behavior of ω_q and Z_q. The results of these calculations, together with a discussion of the form of the dispersion relation at long wavelengths, are presented elsewhere.[6,18]

The approach we have described here is thus seen to provide a consistent account of the single-phonon excitation spectrum of ^{4}He for $q \lesssim 2.1$ Å^{-1} at all pressures in the limit of low temperatures. We find that the
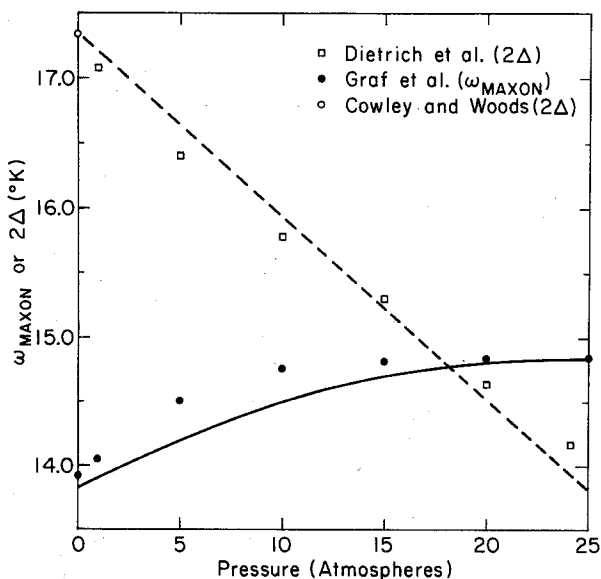

Fig. 5. Roton and maxon energies as a function of pressure; the experimental prints are taken from Graf et al.,[13] Dietrich et al.,[14] and Cowley and Woods.[1]

scalar polarization potential plays a major role in determining this excitation spectrum and that to a good degree of approximation it resembles closely the experimentally determined interaction between ^{4}He atoms, with the principal "liquid" effect coming through the screening of the hard-core part of that interaction by short-range atomic correlations, a screening which is pressure sensitive. It is, however, necessary that one allow as well for both mass polarization effects and the role of the multiparticle excitations, and these play an increasingly important role in determining the excitation spectrum as one goes to wave vectors beyond the maxon region.

In particular, examination of the importance of the various polarization parameters in determining ω_q and Z_q shows that the maxon energy is sensitive to both mass polarization and multiparticle effects, while the roton energy is influenced mainly by the vector polarization potential. The essential nature of the rotons and maxons is still present if one takes $m_q^* \cong 2.7 m_0$, say, and neglects multiparticle excitations, but the resulting energies are far from accurate. On the other hand, the theoretical expression for Z_q is found to be sensitive mainly to the choice of α_q and $\mathscr{A}_q$, that is, to the influence of multiparticle excitations.

Obviously, the phenomenological theory presented here is no substitute for a complete microscopic theory of the excitation spectrum; however, we believe that a polarization potential approach in which due account is taken of mass polarization and multiparticle excitations describes the principal physical effects which must appear in any complete microscopic theory and that the form of the $\chi(q\omega)$ calculated in such a theory will closely resemble our basic expression, Eq. (3). In the present treatment, we have neglected the frequency dependence of the multiparticle contribution to $\chi_{sc}(q\omega)$ and we are currently exploring ways to take that into account, as well as ways to extend the theory to higher temperatures.

ACKNOWLEDGMENT

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