We propose a new theoretical approach to the excitation spectrum of superfluid $^4$He. It is based on the assumption that, in addition to the usual Feynman density fluctuations, there exist localized modes which describe the short range behavior in the liquid associated with microscopic cores of quantized vortices. We describe in a phenomenological way the hybridization of those two kinds of excitations and we compare the resulting energy spectrum with experimental data, e.g. the structure factor and the cross section for single quasi-particle excitations. We also predict the existence of another type of excitation interpreted as a vortex loop. The energy of this mode agrees both with critical velocity experiments and high energy neutron scattering. In addition we derive a relation between the condensate fraction and the roton energy and we calculate the reduction of the ground-state energy due to the superfluid order.

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**I. INTRODUCTION**

In this paper we present an alternative description of the energy spectrum of superfluid $^4$He. Among the standard approaches to this problem, we mainly find either the effective Hamiltonian of Bogoliubov, or the variational approach proposed by Feynman.

The Bogoliubov description relies on the assumption of a weakly interacting Bose gas. Its main success was to obtain a linear dispersion for the long wavelength excitations starting from the quadratic spectrum of free bosons. This linear phonon branch cannot be obtained from simple perturbation theory but corresponds to a RPA-like description of this problem. This linear behavior is indeed one of the main features of the experimental spectrum (fig.1). Nonetheless this success, neither the initial interpretation of the excitations as density fluctuations (phonons) nor the rest of the spectrum beyond the linear part, is quantitatively obtained from this approach.

A alternative description was proposed by Feynman, based on a variational form of the wavefunction for the low-lying excited states which leads to an excitation spectrum of the form

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2mS(k)}$$

where $m$ is the mass of the atoms and $S(k)$ is the static structure factor of the liquid. This expression, using the experimental structure factor, is shown in fig.1. It reproduces quantitatively the low momentum linear behavior, since in this limit the f-sum rule is exhausted by these density fluctuations. Unlike the weakly interacting Bose gas limit, it also reproduces qualitatively the roton minimum. Despite these successes, this variational wavefunction, although it includes Bose symmetry, does not contain special features characterizing the superfluid phase. For instance, since it contains only information about the static structure factor, it gives essentially the same energy spectrum both below $T_\lambda$ in the superfluid phase and in the normal phase ($T > T_\lambda$) where experimental results exhibit very different behaviors for the spectrum of these two phases. Unlike $S(k)$ which almost does not change, the dynamical structure factor $S(k,\omega)$ is very sensitive to the superfluid transition. This shows up in the vanishing of the roton and maxon peaks above $T_\lambda$.

In order to get a better quantitative agreement in the roton region, subsequent refinements of the original variational wavefunction were proposed, which include more localized structure on top of the delocalized density fluctuations (phonons). This was achieved by introducing more variational parameters, at the expenses of the initial interpretation of the excitations as density fluctuations. Despite sizeable improvements for the energy spectrum and other measurable quantities including the scattering intensity, this approach does not fully answer the question of the nature of the superfluid behavior.

An alternative approach to the superfluidity of $^4$He using path integral Monte Carlo calculations was proposed. Although it does not provide explicit results for the spectrum, it showed unambiguously how superfluidity is related to the coherent exchange of atoms along rings of all sizes.

Our motivation in order to build a phenomenological model for the superfluid is based on the features discussed previously. We assume that the main features of superfluidity show up in the spectrum in the large momentum range above the linear phonon part. This includes the roton minimum (at energy $\Delta$) and the saturation for very large $k$'s at the energy $2\Delta$. We propose to view superfluid $^4$He as the condensation in one state of a set of localized states with long-range interactions. This is in contrast to the model of hard-core bosons on a lattice without interactions. We shall describe these local modes as two-level systems (TLS) of bare energy $E_0$. This approach is analogous to the description of dipolar...
The TLS we consider are localized on atomic scales and may correspond to quantum coherent rings of a few atoms only, which are supposed to be responsible for the superfluid behaviour of the liquid. These short rings correspond to vortex cores of sizes $R \simeq 1\text{Å}$, and may be considered as local dipoles. Large ring structures arise from the long-range interaction between the TLS.

The effective Hamiltonian $H_{\text{loc}}$ we propose for these interacting local modes can be diagonalized by a Bogoliubov transformation. The resulting spectrum bears similarity with the weakly interacting Bose gas expression, although it does not assume a weak interaction. Indeed, in order to recover a gapless phonon branch at low momentum ($k \simeq 0$), we need to consider strong interactions, namely interactions of the order of the bare energy $E_0$. Unlike ordered structures of dipoles on a lattice for which it is possible to calculate the interaction term, for liquid $^4\text{He}$ (and for glasses), the interaction term is obtained from the experimental energy spectrum. Despite this shortcoming, this model gives closed analytical expressions for quantities such as the scattering intensity of neutrons by single quasiparticle excitations, the relative variation of the ground-state energy and the condensate fraction in terms of a single quantity, namely the strength of the interaction, so that it becomes possible to relate them.

In order to compare this approach to the Feynman variational scheme, we use an equivalent formulation of our model based on a description of the interaction between the localized modes as due to a virtual exchange of Feynman phonons. This is very much in the way Hopfield and Anderson considered the exciton problem in dielectric media. This description is equivalent to the previous one based on the effective Hamiltonian $H_{\text{loc}}$ provided we use the dipolar approximation which corresponds to large momentum. For low momentum, both the density fluctuations and the large scale exchange cycles correspond to the same degrees of freedom and cannot be disentangled anymore. In the large momentum limit the energy spectrum results from the hybridization of these two kinds of excitations, which represent independent degrees of freedom of the superfluid. This way we gain a better understanding of the roton part of the spectrum. In addition we find a new localized excitation branch at energy $E_2 = 2E_0$, which we interpret as microscopic vortex-loop excitations of the superfluid. These type of excitations are usually thought as being completely independent of the phonon-roton excitations, while here we propose a model that describes them both together.

This paper is organized as follows. We begin by introducing the effective Hamiltonian of the strong coupling description in section II. In section III, we obtain expressions for the scattering intensity of the single-excitation branch and compare it to the experimental data. In section IV, we evaluate the reduction in the ground-state energy of the superfluid and the condensate fraction. In section V, we consider the dipolar approximation and the resulting hybridization scheme. We compare the resulting spectrum and the static structure factor to the experimental data. Finally, in section VI, we discuss the vortex-loop branch and we conclude in section VII.

### II. THE EFFECTIVE HAMILTONIAN DESCRIPTION

We consider superfluid $^4\text{He}$ as a set of local states described as two-level systems of bare energy $E_0$. Their Hamiltonian is then

$$H_{\text{loc}}^0 = \sum_k E_0 b_k \dagger b_k$$  \hspace{1cm} (2)

where translational invariance allows us to write operators in $k$-space. The operators $b_k$ obey bosonic commutation relations. This holds in the limit of a low density of localized modes, i.e. for the case of no multiple occupation of a site. This condition corresponds to vortex-cores or small exchange rings which cannot be multiply excited on the same site. The value of $E_0$ will be determined later on.

The interaction between these localized modes can generally be written as

$$H_{\text{loc}} = \sum_k (E_0 + X(k)) b_k \dagger b_k$$ \hspace{1cm} (3)

$$+ \sum_k X(k) \left( b_k \dagger b_k + b_k b_k \right)$$

The diagonal part in this Hamiltonian corresponds to the hopping of a local mode between sites, and the off-diagonal part describes the creation (or the annihilation) of pairs of local modes on distinct sites. The matrix element $X(k)$ depends on the microscopic details of the interaction. For a lattice structure like excitons in a crystal or solid $\text{bcc}^4\text{He}$, it is possible to express $X(k)$ as a summation of dipolar terms. This is not possible in the superfluid phase, for which we have no lattice structure.

The Hamiltonian $H_{\text{loc}}$ is diagonalized by the Bogoliubov transformation $\beta_k = u(k) b_k + v(k) b_k \dagger$. The resulting spectrum is

$$E(k) = \sqrt{E_0(E_0 + 2X(k))}$$ \hspace{1cm} (4)

and the two functions $u(k)$ and $v(k)$ are given by

$$u^2(k) = \frac{1}{2} \left( \frac{E_0 + X(k)}{E(k)} + 1 \right)$$

$$v^2(k) = \frac{1}{2} \left( \frac{E_0 + X(k)}{E(k)} - 1 \right)$$ \hspace{1cm} (5)
The corresponding ground-state wavefunction for the local modes is

$$|\Psi_0\rangle = \prod_k \exp \left( \frac{m_k}{u_k} b_k^\dagger b_{-k}^\dagger \right) |\text{vac}\rangle \quad (6)$$

where $|\text{vac}\rangle$ is the state with no local modes, i.e. annihilated by $b_k$, namely $b_k |\text{vac}\rangle = 0$. The ground-state is a coherent state of pairs of localized-modes. This coherent state defines a global phase which, once fixed, breaks the gauge-invariance. The excitation given by $|\beta^\dagger_k |\Psi_0\rangle$ corresponds to the breaking of a pair of momentum $k$, leaving an unpaired local-mode.

The expressions of the bare energy $E_0$ and $X(k)$ stem from the following remarks. The equality $E(k) = E_0$ is achieved in the zero coupling limit ($X(k) = 0$) and it corresponds to a normal phase for the local modes characterized by $v_k = 0$ in the relations (6) and (9). This corresponds to the termination point of the energy spectrum for which, at large momentum $k$, the energy goes to $2\Delta$ where $\Delta$ is the roton energy (fig.1). Beyond the termination point, there is no quasi-particle excitation and only a structureless free-recoil scattering characteristic of a normal liquid. We shall therefore take for the bare energy the value $E_0 = 2\Delta |\Psi_0\rangle$.

In the opposite limit, i.e. for low momentum $k \to 0$, we demand that the spectrum (6) will be gapless, namely $E(0) = 0$. This requires

$$X(0) = \frac{E_0}{2} = -\Delta \quad (7)$$

Notice that for dipoles on a lattice, this condition is a self-consistent definition of $E_0$ since the energy required to excite locally a dipole from the ground-state corresponds to the one needed to flip it with respect to the coherent background. This excitation changes the sign of the interaction energy and costs $2 |X(k)| = 2\Delta = E_0$, which corresponds to the previous definition of the energy of the local mode.

For arbitrary $k$, $X(k)$ is obtained by comparing Eq. (9) with the measured energy spectrum (fig.2). This shape of $X(k)$ is similar to the expression calculated for dipoles on a simple cubic lattice along various directions. This could be helpful towards the development of a microscopic model for the superfluid phase.

It is useful at this stage to compare our approach with the weakly interacting Bose gas limit. There, the Hamiltonian is given within the Bogoliubov approximation by

$$H_{BGB} = \sum_k (\varepsilon_k + N_0 V_k) a_k^\dagger a_k$$

$$+ \sum_k N_0 V_k \left( a_k^\dagger a_{-k}^\dagger + a_k a_{-k} \right) \quad (8)$$

where $N_0 = |\langle a_0 \rangle|^2$, $\varepsilon_k = \hbar^2 k^2 / 2m$, and $V_k$ is the effective potential between the bosons at wave vector $k$. The operators $a_k^\dagger$ and $a_k$ correspond to the creation and annihilation of an atom and not of a localized-mode as in (6).

The Bogoliubov excitation spectrum which corresponds to (6) is

$$E = \sqrt{\varepsilon_k (\varepsilon_k + 2N_0 V_k)} \quad (9)$$

This spectrum is linear in the $k \to 0$ limit ($E \approx \hbar c$), with a sound velocity defined by $c = \sqrt{N_0 V_0 / m}$.

The physics described by the two Hamiltonians $H_{loc}$ and $H_{BGB}$ is very different. The weakly interacting Bose gas has a non-interacting limit given by the ideal Bose gas which, at $T=0$, is known to be fully condensed in the state $k = 0$ and which has already a broken gauge symmetry. The interaction depletes the condensate and changes the spectrum to linear at low momentum. On the other hand, the Hamiltonian $H_{loc}$ corresponds to a set of independent localized modes with no broken symmetry in the non-interacting limit ($X(k) = 0$). To restore in the linear momentum regime both the condensation and broken gauge symmetry, we need a non-zero interaction $X(k)$. Since this interaction is large ($X(0) = -E_0 / 2$), it is not a small perturbation to the non-interacting case. In that sense, it is a strong-coupling description of the superfluid.

We would like to point out that the entire excitation spectrum given by (6) is unique to the superfluid phase, as only there we can define the function $X(k)$ and local mode energy $E_0$. In particular, the phonon mode is different from the zero-sound mode that appears in the normal fluid. We shall now use this approach to obtain analytical results that we shall compare subsequently with experimental measurements.

### III. SCATTERING INTENSITY

The neutron scattering intensity is a direct probe of the density fluctuations in the liquid and may be described using the dynamic structure factor $S(k, \omega)$. It is usually accepted since the work of Miller, Pines and Nozières that we can split the total contribution to $S(k, \omega)$ into two parts,

$$S(k, \omega) = N Z(k) \delta(\hbar \omega - \varepsilon(k)) + S^{(1)}(k, \omega) \quad (10)$$

where the first term accounts for single quasi-particle excitations of weight $Z(k)$, while the second describes multiparticle excitations. This separation is justified at low temperature and low momentum, typically for $k \lesssim 0.5 \AA^{-1}$. In this regime, integrating (10) over the energy and noticing that $S^{(1)}(k, \omega)$ vanishes in the low momentum limit we obtain $Z(k) = S(k)$, which results also from the Feynman theory. The comparison with the experimental data shows that it works indeed in the low momentum regime mentioned above, but fails to describe the non-linear part of the spectrum, except perhaps for the position of the maximum.

Since the excitations of the local modes from the ground state (6) involve breaking pairs of coherent local
modes, the probability of a neutron to scatter inelastically on such an excitation is proportional to the occupation density of these pairs at each momentum given by $\langle b_k^\dagger b_{-k} \rangle = u_k v_k$, so that

$$Z(k) = 4\pi k^2 I_0 u_k v_k$$

where $I_0$ is an arbitrary normalization constant and where the factor $4\pi k^2$ comes from the three dimensional phase space. Using the expression (11) for $u_k$ and $v_k$, we obtain $u_k v_k = \frac{1}{\pi k^2 E_0} |X(k)|^2$ which together with (9) gives

$$Z(k) = \frac{4\pi k^2 I_0 E_0}{E(k)} \left( \frac{E(k)}{E_0} \right)^2 - 1$$

Using the experimental $E(k)$ in expression (12) we obtain a differential cross section which agrees well with the experimental results obtained at saturated vapor pressure (S.V.P.) as shown in fig.3. In the low momentum limit, we recover the proportionality between $S(k)$ and $Z(k)$ and therefore $Z(k)$ is linear with $k$. We emphasize that as a result of both (12) and the saturation of $E(k)$ to $2\Delta$ at large $k$, the scattering intensity $Z(k)$ vanishes identically at this point. This indeed corresponds to the experimental measurement of $Z(k)$, and could not be obtained neither from weakly interacting Bose gas description nor by variational approaches.

**IV. DESCRIPTION OF THE CONDENSATE**

**A. Condensate fraction**

In the microscopic description of a Bose liquid, the condensate is usually characterized by the condensate fraction, $n_0/n$, which measures the relative occupation by the atoms of the lowest energy state. At zero temperature it is equal to one for an ideal Bose gas, while a finite interaction depletes the lowest energy state with temperature it is equal to one for an ideal Bose gas, while the second term in (16) is the shift in the ground state occupation number $n_k = v(k)^2$ of the local modes. Using (13), it is given by

$$n_k \rightarrow 0 = \frac{\Delta}{2\hbar c}$$

Since both (13) and (14) describe the same behaviour, namely the condensation of the $^4$He atoms, then, by equating the two corresponding residues, we obtain the relation

$$\frac{n_0}{n} = \frac{\Delta}{mc^2}$$

This relation predicts a direct and unexpected link between the condensate fraction $n_0/n$ and the characteristics of the energy spectrum at $T = 0$, namely the sound velocity $c$ and the roton energy $\Delta$. The behavior of both $n_0/n$ and $\Delta/(mc^2)$ measured as a function of the pressure are in agreement with the relation (17) up to a factor of nearly two which we shall discuss later on.

Another relevant feature of (17) is that it allows to relate the quantity $n_0/n$ which is critical at the superfluid transition and therefore is proportional to the amplitude of the complex order parameter, to the roton energy $\Delta$ which, in our model, is the modulus of the interaction matrix element at $k = 0$ namely $|X(k = 0)| = \Delta$. A critical behavior of $\Delta$ was indeed recently observed in high resolution neutron scattering experiments, and supported by Raman scattering experiment. This seems to indicate that the roton energy $\Delta$ (and therefore the interaction matrix element $X(k)$) is related to the superfluid order as it appears in (17).

**B. Condensation energy**

Another quantity which characterizes the condensate is the condensation energy $\Delta E_G$. It is obtained by rewriting $H_{loc}$ in (9) in terms of the operators $\beta_k$ and $\beta_k^\dagger$, namely

$$H_{loc} = \sum_k E(k)\beta_k^\dagger \beta_k + \sum_k \frac{1}{2} (E(k) - (E_0 + X(k)))$$

where $c$ is the sound velocity and $m$ is the mass of a $^4$He atom. For the real liquid, we do not know how to obtain $n_0/n$ in terms of other measurable quantities. This ratio has been obtained indirectly from a measurement of the distribution of the non-condensed atoms. Numerically, using path integral Monte-Carlo similar values have been obtained. An analytical expression has been proposed which is based on the assumption that the depletion of the condensate is related to the thermally excited rotons.

In the present model, it is also possible to obtain the divergent part of the ground state occupation number $n_k = v(k)^2$ of the local modes. Using (3), it is given by

$$n_k \rightarrow 0 = \frac{\Delta}{2\hbar c}$$

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$$H_{loc} = \sum_k E(k)\beta_k^\dagger \beta_k + \sum_k \frac{1}{2} (E(k) - (E_0 + X(k)))$$

The second term in (17) is the shift in the ground state energy $\Delta E_G$. Using Eq.(4) we obtain

$$\Delta E_G = \frac{1}{8\Delta} \sum_k (E(k) - 2\Delta)^2$$

or

$$\Delta E_G = \frac{V_{sp}}{32\pi^2 \Delta} \int_0^{k_{max}} k^2 (E(k) - 2\Delta)^2 dk$$

This relation predicts a direct and unexpected link between the condensate fraction $n_0/n$ and the characteristics of the energy spectrum at $T = 0$, namely the sound velocity $c$ and the roton energy $\Delta$. The behavior of both $n_0/n$ and $\Delta/(mc^2)$ measured as a function of the pressure are in agreement with the relation (17) up to a factor of nearly two which we shall discuss later on.

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where \( k_{\text{max}} \) is the largest value of the momentum and corresponds to the termination point of the quasi-particle spectrum. \( V_{sp} \) is the specific volume per atom. Using the experimental (fig. 1) energy spectrum for \( E(k) \), we obtain

\[
\Delta E_G \simeq -5.0 \pm 1.0K(SVP)
\]
\[
\Delta E_G \simeq -3.0 \pm 1.0K(P = 24atm)
\]

(19)

for saturated vapor pressure and \( P=24\text{atm} \) respectively. In fig. 4 we plot the integrand \( k^2(E(k)-2\Delta)^2 \) in (18). It shows that the main contribution to the reduction in the ground state energy comes from the roton part of the spectrum due to the larger phase space volume, compared with the phonon region \( (k \rightarrow 0) \).

Both from experimental data (2) and path integral Monte-Carlo calculations (23), it is possible to deduce the values for the change in the kinetic zero point energy of the atoms between the normal phase at \( T_\lambda \) and the superfluid phase in the limit \( T \rightarrow 0 \)

\[
\Delta E_{kin} \simeq 2.5 \pm 3.0K(SVP)
\]
\[
\Delta E_{kin} \simeq 1.3 \pm 3.0K(P = 24atm)
\]

(20)

for saturated vapor pressure and \( P=24\text{atm} \) respectively. First, we notice that the large experimental uncertainty makes any quantitative comparison difficult. Moreover, the two quantities \( \Delta E_G \) and \( \Delta E_{kin} \) do not measure exactly the same property. While \( \Delta E_G \) measures the change in the ground state energy of the local modes between the non-interacting and interacting limits, both at \( T=0 \), \( \Delta E_{kin} \) measures the change in kinetic energy per atom between two different temperatures. Since the variation of the volume of the superfluid between \( T_\lambda \) and \( T=0 \) is small (4), it is usually accepted to attribute the change in the kinetic energy mainly to the condensation phenomenon. In our model this condensation energy is calculated per local mode, nevertheless we find that both quantities decrease for an increasing pressure.

C. Effective mass

Although the relations (15) and (18) for the condensate fraction and the condensation energy give both the right order of magnitude and the expected behaviour as a function of pressure, they are consistently larger than the experimental values by a factor of about 2. This factor may stem from the fact that our expressions are given as a function of the local modes while the experimental data is obtained per \(^4\text{He} \) atom, and there is no direct one-to-one correspondence between these two. Therefore, the mass term which appears in (15) instead of being the bare mass \( m \) of a \(^4\text{He} \) atom is the effective mass \( m_{eff} \) of the bare local mode. From the above comparison between \( n_0/8 \) and \( \Delta E_G \) with experiments we obtain that \( m_{eff} \approx 2m \). Although such a relation can be obtained only from a microscopic calculation beyond our phenomenological model, it is interesting to notice that a similar result was obtained numerically using path integral Monte-Carlo calculations (23). There, the effective mass \( m^* \) of a tagged \(^4\text{He} \) atom which does not participate in the Bose permutations was found to be \( m^* \approx 2m \). Since such a tagged atom is a local node or defect in the superfluid, it corresponds to the bare local mode we consider in the Hamiltonian \( H_{loc} \). As we saw in (15) and (18), the bare local mode of energy \( E_0 \) appears for the non-interacting case \( (X(k)=0 \) and \( v(k)=0) \). Then, it does not contribute to the coherent (superfluid) ground state, i.e. behaves as a local node of the order parameter. This correspondence may justify taking \( m_{eff} \approx 2m \) bringing both (15) and (18) into agreement with the experimental data represented in fig. 5, where the experimental values (27) for \( n_0/n \), \( \Delta \) and \( c \) are obtained independently (22).

V. HYBRIDIZATION OF LOCALIZED AND DENSITY MODES

In the previous sections we described the superfluid as resulting from the condensation of a set of localized and interacting modes in the strong coupling limit. This description, as we emphasized, is very different from the Bogoliubov weak coupling limit. Since it is aimed to describe the full energy spectrum, we would like to relate it to the Feynman variational scheme. In this section we shall show that in addition to the phonon-roton branch of excitations around the roton momentum, there is another branch of excitations. We shall discuss the properties of this excitation in the light of experiments on thermal nucleation of vortices (22) and on large momentum neutron scattering (24). To that purpose, we propose in this section a description equivalent to the previous interacting local mode problem, where the interaction between these modes results from the exchange of virtual photons. This is very much in the same spirit of Hopfield (25) and Anderson considering the exciton problem in dielectric media. There localized excitons, taken as dipoles, interact through the exchange of photons. For the superfluid, the local modes play the role of the excitons, and interact through the exchange of Feynman phonons. This picture is only valid in the range of large enough momentum beyond the linear part around \( k \rightarrow 0 \), which corresponds to density excitations (i.e. Feynman phonons). It is only in this regime that the two types of excitations represent independent degrees of freedom of the system. The Hamiltonian describing Feynman density excitations is

\[
H_0 = \sum_k \varepsilon(k) a_k^\dagger a_k
\]

(21)

where \( a_k \) are Bose operators and \( \varepsilon(k) \) is the Feynman spectrum given by the relation (16), expressed in terms of the static structure factor \( S(k) \). The Hamiltonian describing the coupling between these phonons and the localized modes is (16).
where \( H_c = \sum_k (\lambda(k, E_0)b_k + \mu(k, E_0)a_k)(a_k^\dagger + a_{-k}) \) (22)

and the total Hamiltonian is

\[ H = H_0 + H_0^0 + H_c \] (23)

Since \( H \) and \( H_0^0 \) provide two equivalent descriptions of the same problem, the functions \( \lambda \) and \( \mu \) are related to \( X(k) \). If we now assume that the localized modes are local dipolar excitations, then there is a specific relation between these functions, given by \( \lambda(k) = iE_0 \left( \frac{3X(k)}{2\epsilon(k)} \right)^\dagger \) and \( \mu(k) = -E_0 \frac{3X(k)}{2\epsilon(k)} \).

As we shall discuss later on, this dipolar approximation is valid only for large momentum, i.e. in the roton region. The two modes \( a_k \) and \( b_k \) are independent degrees of freedom, so that their commutator is zero. The total Hamiltonian can be diagonalized using the canonical transformation

\[ \alpha_k = A(k)a_k + B(k)b_k + C(k)a_{-k}^\dagger + D(k)b_{-k}^\dagger \]

\[ \hat{\alpha}_k = B(k)a_k + A(k)b_k + D(k)a_{-k}^\dagger + C(k)b_{-k}^\dagger \]

which describe respectively the lower and upper branch of the energy spectrum. The functions \( A(k), B(k), C(k), D(k) \) can be written down explicitly.

We point out that the roles of the phonons and localized-modes are interchanged between the two branches, as can be seen by writing the ground-states of both branches:

\[ |0_1\rangle = \prod_k \exp \left( \frac{C(k)}{A(k)}a_{-k}^\dagger a_{-k} \right) \exp \left( \frac{D(k)}{B(k)}b_{-k}^\dagger b_{-k} \right) \]

\[ |0_2\rangle = \prod_k \exp \left( \frac{D(k)}{B(k)}a_{-k}^\dagger a_{-k} \right) \exp \left( \frac{C(k)}{A(k)}b_{-k}^\dagger b_{-k} \right) \] (25)

The corresponding dispersion relation is

\[ [E^2(k) - \varepsilon^2(k)] [E^2(k) - E_0^2] = -6X(k)E_0E^2(k) \] (26)

We first notice that for a vanishing coupling \( X(k) = 0 \), we obtain, as expected, the two solutions \( E_1(k) = \varepsilon(k) \) and \( E_2 = E_0 \), describing respectively pure density and non-interacting localized modes. A non-zero coupling hybridizes these two sets of excitations. Since \( X(k) \) and \( E(k) \) are also related by the relation

\[ E^2(k) - E_0^2 = 2X(k)E_0 \] (27)

using the relations (24) and (26), we obtain a two branch spectrum of dispersions

\[ E_1(k) = \frac{1}{2} \varepsilon(k) = \frac{\hbar^2 k^2}{4mS(k)} \]

\[ E_2 = 2E_0 = 4\Delta \] (28)

These expressions are written in terms of \( \varepsilon(k) \) and \( \Delta \), but they depend also explicitly on \( X(k) \) through [4], which is a consequence of the dipolar approximation. As a result of the hybridization, the energy spectrum \( E_1(k) \) of the density fluctuations is shifted by a factor 2 towards lower energies relatively to the Feynman ansatz. There is in addition a new branch \( E_2 \) of localized excitations at a constant energy which is twice the value of the bare local mode.

It is of some interest to notice that it is possible to express the factors \( \frac{C(k)}{A(k)} \) and \( \frac{D(k)}{B(k)} \) appearing in the coherent ground-state wavefunctions of the two branches in terms of the energies, namely

\[ \frac{C(k)}{A(k)} = \frac{\varepsilon(k) - E(k)}{\varepsilon(k) + E(k)} \]

\[ \frac{D(k)}{B(k)} = \frac{E_0 - E(k)}{E_0 + E(k)} \] (29)

For the special value \( k = k_{\text{rot}} \) which corresponds to the roton minimum, they are both equal, \( |C/A| (k_{\text{rot}}) = |D/B| (k_{\text{rot}}) = 1/3 \), a consequence of the relation (28).

The roton excitation then appears as involving the maximum mixing of localized and density modes in equal proportions.

We want now to compare these results with the experimental data [21] obtained for the energy spectrum \( E(k) \) (fig.6) and for the structure factor \( S(k) \) at two different pressures (fig.7). Around the roton minimum, and over quite a large range of momentum, the relation (28) is in good agreement with the experimental results and gives a spectrum which is reduced from the Feynman result by a factor of nearly two. It is interesting to recall that Feynman himself in his original paper [4] noticed the factor 2 discrepancy between his ansatz and the experimental results around the roton minimum. Here we deduce it from a closed analytical solution. This interpretation of the roton excitation as resulting from the dipolar hybridization of two separate excitations is to be compared with the approach of Glyde and Griffin [32,42] which uses a dielectric formalism to describe hybridized phonons and free-particle excitations. The main discrepancy is obtained in the low momentum region \( k \leq 1A^{-1} \), i.e. below the maxon momentum. As \( k \to 0 \) the experimental data is close to the Feynman result i.e. twice the value we obtain in (28). This regime is beyond the dipolar approximation we consider and sets the limit of validity of this approach. To be able to describe the linear phonon regime from the present approach, we should include multipoles terms.

VI. HIGH ENERGY EXCITATION BRANCH

A. Vortex loops

The relation (28) gives a second branch of excitations at the constant energy \( E_2 = 4\Delta \). It describes a localized (dispersionless) excitation of energy which is twice the bare vortex core (local mode) energy. The intuitive
physical picture of this mode is therefore of an excitation made out of two vortex-core excitations. Such an excitation in three dimensions may be viewed as a microscopic vortex-loop, or a localized defect. The radius \( R \) of a vortex-loop can be estimated using a Feynman-type formula for the energy of the associated circulating current \( E_{\text{vortex}} \):

\[
E_{\text{vortex}} = 2\pi^2 \rho \frac{h^2 R}{m^2} \ln \left( \frac{R}{a} \right)
\]  

(30)

where at \( T = 0 \), we take the density of the superfluid \( \rho \) to be the total density \( \rho \) and \( a \) is the core size equal to the atomic radius namely \( a \simeq 1.44 \text{Å} \). The radius \( R \) obtained from (30) and which corresponds to \( E_{\text{vortex}} = 4\Delta = 34.4K \) is \( R \simeq 5.1A \).

Experimental support for the interpretation of the hybridized localized state at \( E = 4\Delta \) as an intrinsic excitation of the fluid is provided by critical velocity experiments. In phase-slippage studies of the critical velocity through an orifice, the critical velocity is driven by the thermal nucleation of vortex-loops. The corresponding activation energy \( E_v \) is determined by the nucleation rate \( \Gamma \) given by the Arrhenius law \( \Gamma = \Gamma_0 \exp \left( \frac{E_v}{k_BT} \right) \) and turns out to be \( E_v \simeq 33 \pm 5K \) a value indeed very close to \( 4\Delta = 34.4K \). Moreover, the upper critical velocity \( v_c \) may be estimated to be the velocity of the vortex-loop itself \( \frac{h}{2\pi n} \) i.e. \( v_c = \frac{h}{2\pi n} \ln \left( \frac{R}{a} \right) \simeq 20m/s \), a value close to the largest measured critical velocity \( \frac{h}{2\pi n} \).

Finally, recent experiments on cavitation in superfluid \(^4\text{He} \) are analyzed in terms of thermal a nucleation process. The activation energy found is of the order of \( 4\Delta \), indicating a possible connection between a microscopic vortex-loop and the thermal nucleation of caviton.

We also point out that this interpretation of the vortex-loop branch as distinct from the phonon-roton branch is further supported experimentally by ion velocity measurements and theoretically using hydrodynamic methods.

**B. High energy neutron scattering**

Recent high resolution neutron scattering data show that at high energy and momentum transfer, compared with the phonon-roton branch, the position of the scattering peak is consistently at a lower energy than the free-recoil value. At such high energies the atoms of the liquid behave freely and therefore with a quadratic dispersion \( E_{\text{free}}(k) = \frac{h^2 k^2}{2m} \). There is a marked broadening of the width of this peak where the free-recoil spectrum crosses the second branch of energy \( 4\Delta \) at momentum \( k_c \simeq 2.3\text{Å}^{-1} \). This data can be understood as resulting from the superposition of the free-recoil spectrum and the process of vortex-loops creation. Such a possibility for explaining the increased width of the dispersion curve using vortex-loop creation was suggested by Cowley and Woods. A recoiling atom can create vortex-loops and lose the corresponding energy and momentum, so that its remaining energy is

\[
E_n(k) = 4n\Delta + \frac{h^2}{2m} (k - k_{c,n})^2
\]

(31)

where \( n \) is the number of emitted vortex-loops and \( k_{c,n} \) is given by the equality of the free-recoil energy and the \( n \)th vortex-loop energy, so that \( k_{c,n} \simeq 2.3\sqrt{n} \text{Å}^{-1} \). We show the dispersion for the first two emitted vortex-loops in fig.8. Then, by subtracting from the experimental neutron-scattering data a Lorentzian centered around the free-recoil energy and fitted to the highest energy tail, we find an additional scattering peak around the energy given by (31). In fig.9 the experimental results are plotted, which correspond to \( k \)'s such that \( n = 1 \) or 2. At higher energy transfer the free-recoil spectrum can be split again at twice \( 4\Delta \) and so on, as is indicated in fig.9d.

There is a series of such splittings each time the recoiling atom has an energy which is an integer multiple of \( 4\Delta \). In fig.10, the experimental results for the high momentum transfer \( k = 10\text{Å}^{-1} \) are shown. At this momentum the free-recoil energy is more than 17 times the vortex-loop energy of \( 4\Delta \), and we find that the extra scattering is well described as a ‘band’ of splitted levels below the free-recoil spectrum.

### VII. CONCLUSION

In this paper, we have presented a phenomenological strong coupling theory for the superfluid phase of \(^4\text{He} \) in order to describe features that correspond to excitations of energies beyond the phonon part of the spectrum. This approach is based on the assumption that at short length scales, there exists a set of interacting localized excitations. This is very much in the spirit of the assumption of two-level tunneling states in dielectric glasses. These excitations are described by an effective Hamiltonian which depends on the strength \( X(k) \) of the interaction between these modes. We used experimental results obtained in neutron scattering in order deduce the behaviour of \( X(k) \). This approach gives a hand to calculate analytical expressions for various physical quantities like the scattering cross-section \( Z(k) \) for single particle excitations, and the shift in the ground state energy. In addition, it allowed us to derive a relation between the condensate fraction and characteristics of the energy spectrum namely the sound velocity and the roton energy \( \Delta \). This gives a way to measure directly the condensate fraction. Moreover, it establishes the critical nature of \( \Delta \) and its relation to superfluidity in close connexion with recent experimental results. Then, we derived an alternative description of the set of localized modes which allowed us to predict the existence of a new branch of excitations at energy \( 4\Delta \) beyond the phonon-roton branch. This branch which has...
not yet been observed directly and allows to interpret phase slippage experiments and to get a hint for the puzzling broadening observed at high energy and momentum transfer neutron scattering. Since we interpret this excitation as the smallest vortex-loop (or local defect) of the superfluid, our model offers a way of describing both the phonon-roton and the localized vortex-loops within one scheme.

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FIG. 1. The experimental energy spectrum at saturation vapor pressure [3,9,32] compared with the Feynman phonon spectrum (Eq.1) based on the experimental static structure factor $S(k)$ [33-35]. Also marked is the roton energy $\Delta$ and the termination of the quasi-particle branch at energy $2\Delta$ (circled point).

FIG. 2. The interaction matrix $X(k)$ from Eq.(4), based on the experimental energy spectrum at (a) saturation vapor pressure [3,9,32] and (b) $P=24$ atm [3]. The bare energy of the local mode is taken to be $E_0 = 2\Delta$. Notice that $X(k)$ tends to zero at the termination point of the spectrum at high momentum.
FIG. 3. Comparison between the experimental scattering cross-section \(Z(k)\) of single quasi-particle excitations (points) at 1.1K and the theoretical curve (solid line), obtained using the experimental data for the energy spectrum at saturated vapor pressure \(E(k)\) \([3,9,32]\) in Eq.(12).

FIG. 4. The integrand \(k^2 (E(k) - 2\Delta)^2\) appearing in the calculation of the reduction in the ground state energy \(\Delta E_G\) in Eq.(18). (a),(b) are at saturation vapor pressure and \(P=24\)atm respectively. Notice the large contributions around the roton momentum.
FIG. 5. Comparison between the experimental condensate fraction at different densities (solid circles) [23] and Eq. (15), using an effective mass for the local modes of \( m_{\text{eff}} = 2.3m \) (solid line).

FIG. 6. Comparison between the experimental energy spectrum [3,9,32] (points) and the energy \( E_1(k) \) in Eq. (28) (solid line), where the structure factor \( S(k) \) is obtained from independent measurements [33-35]. (a) and (b) correspond respectively to the saturation vapor pressure and to \( P=24 \) atm. The dashed line at energy \( E_2 = 4\Delta \) indicates the position of the localized branch of excitations (vortex-loop).
FIG. 7. Comparison between the experimental structure factor $S(k)$ [33-35] (solid circles) and expression Eq.(28) (solid line) for the same two pressures as in Fig.6, where the energy $E(k)$ is obtained from independent measurements [3,9,32].

FIG. 8. The dispersion relations of the free recoil ($n = 0$) and the lowest two levels of recoiling atoms that correspond to vortex-loops emission ($n = 1, 2$) (Eq.31).
FIG. 9. Comparison between the experimental scattering profiles [29] (solid circles) and the free-recoil Lorentzian (heavy dashed-line) at different momenta: (a) $k = 2.8\,\text{Å}^{-1}$, (b) $k = 3.0\,\text{Å}^{-1}$, (c) $k = 3.2\,\text{Å}^{-1}$, (d) $k = 4.0\,\text{Å}^{-1}$. The remaining extra scattering is the heavy solid-line. The vortex-loop energy ($4\Delta$) is indicated by the vertical dotted-line, the free-recoil energy by the vertical long-dashed-line, and the $n = 1$ splitted energy Eq.(31) by the vertical dashed-dot line. At relatively low momenta (a,b) there is still a noticeable phonon-roton peak around the $2\Delta$ energy. In (d) the heavy vertical lines indicate the $n = 2$ vortex-loop emission by the recoiling atom.

FIG. 10. (a) Experimental scattering profile [44] at $k = 10.0\,\text{Å}^{-1}$ (solid circles). The free-recoil Lorentzian (heavy dashes-line) and extra scattering (heavy solid-line) are plotted. The free-recoil energy is indicated by the long-dashed vertical line. (b) The spectrum of the free-recoil (dash-dot) and the 17 splittings due to vortex-loop excitations (Eq. 31) (alternating solid and dashed lines).