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Is the roton in superfluid ${}^4\text{He}$ the ghost of a Bragg spot?

Philippe Nozières

Laboratoire d'Etude des Propriétés Electroniques des Solides;
Centre National de la Recherche Scientifique,
B.P.166, 38042 Grenoble Cedex9

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Abstract

It has always been assumed that the roton in ${}^4\text{He}$ had to do with local vorticity - hence the name! We present here an alternate view: the roton is viewed as a "soft mode", precursor of a crystallization instability. In such a picture the liquid is "nearly solid", and the long observed similarities of heat propagation in liquid and solid phases are naturally explained. In this qualitative paper we consider three models successively. A lattice gas with one atom per site displays a Mott localization transition, as shown by the Bangalore group. The important result is the vanishing of the superfluid order parameter (condensate fraction N_o) at the transition. There is no breakdown of translational symmetry and consequently no soft mode. Another lattice model with half filling, with an added nearest neighbour repulsion, was studied by Matsubara and Matsuda in the early fifties: it displays a first order transition between a superfluid and a localized charge density wave state. The excitation spectrum has a soft mode at zone edge near the transition, signalling the proximity of the CDW instability. Finally we consider the realistic situation of a continuous system with no preexisting lattice. We approach the problem from the limit $N_o = 0$ instead of the ideal gas $N_o = N$. When $N_o = 0$ the quasiparticle spectrum and the charge density spectrum are decoupled. The latter should have a soft mode $\omega = \omega_m$ if crystallization is close. That soft mode is a normal state property that has nothing

to do with superfluidity. A small N_o acts to hybridize quasiparticles and density fluctuations: the resulting anticrossing lowers ω_m^2 as well as the ground state energy. We show that N_o is bounded for two reasons: (i) if ω_m^2 turns negative the liquid is unstable towards freezing (ii) depletion due to quantum fluctuation exceeds N_o if the latter is too large. The resulting upper bound for N/N_o is $\ll 1$, a consequence of the deep roton minimum. The whole paper is qualitative, based on outrageous simplifications in order to make algebra tractable.

This paper is dedicated to Prof. David Pines on his 80th birthday

1 Introduction

Ever since the famous work of Landau and Feynman on superfluid ${}^4\text{He}$ it has been argued that the roton minimum is related to local vorticity (hence the name). Feynman coined the beautiful sentence "*a roton is the ghost of a vanishing vortex ring*".[1] Putting flesh on that statement is by no means trivial, as the toroidal geometry of the object is not easily handled. The vortex ring is a metastable topological singularity, which should presumably collapse when its radius R is comparable to its core radius ξ where ξ is the correlation length fixed by the balance of kinetic and potential energies. The energy of such a ring is $N\xi^3 \cdot \hbar^2/m\xi^2$, where N is the particle density and m their mass. Since a typical excitation has an energy $\hbar^2/m\xi^2$ the number of quanta released by the collapsing ring should be $\approx N\xi^3$. For a weakly interacting dilute gas that number is large and the Feynman picture does not apply - but we know there is no roton minimum in that case! For strong coupling $N\xi^3 \approx 1$ and a decay of the ring into a few roton quanta is possible. But how does one relate the energy and momentum of a local structure to that of a plane wave excitation? How can one conserve both with a single quantum? These questions do raise a beautiful theoretical challenge.

Is that challenge relevant to ${}^4\text{He}$? In this note we explore an alternate possibility, where the roton minimum would signal the proximity of solidification. The argument is simplest in a 1d toy model (of course quantum fluctuations preclude real long range superfluid order in 1d: ignore it for a moment). Crystallization is just a charge density wave instability (CDW). The period a contains exactly one particle per lattice site, corresponding to a *localization* transition that is the primary feature. If that transition is second order, we expect a *soft mode*: the excitation spectrum ω_q should have

a dip when q is the reciprocal lattice vector $G = 2\pi/a$. That is indeed what happens in 1d, as shown by modern bosonization techniques[2]. CDW and superfluidity are competing order parameters: if one wins, the loser manifests itself as a soft mode, which does resemble the roton! Unfortunately carrying that argument over to 3d is not trivial as crystallization also implies a breakdown of rotational invariance. While ω_q is isotropic in the liquid phase, it vanishes at discrete Bragg positions in the solid: the resulting transition is first order. As a result the soft mode never vanishes - but it can be well marked as a "roton" dip. If that is so the roton is the "ghost of a Bragg spot"!

In a sense, such a view is implicit in another famous result of Feynman, namely the connection between ω_q and the static form factor

$$NS_q = \int_0^{+\infty} S(q, \omega) d\omega$$

By a series of elegant physical arguments Feynman argues that the excitation spectrum is

$$\omega_q = \frac{q^2}{2mS_q} \quad (1)$$

(we set $\hbar = 1$). A minimum in ω_q corresponds to a maximum in S_q , which in turn signals short range crystalline order. From a naive vantage point, Feynman spectrum relates rotons to crystallization, despite the fact it is only a few pages away from the vanishing vortex ring! In practice the result 1 is only a first approximation, based on the assumption that the dynamic form factor $S(q, \omega)$ has only one discrete peak for each q . We know it obeys the so called "f-sum rule"

$$\int_0^{+\infty} S(q, \omega) \omega d\omega = \frac{Nq^2}{2m}$$

from which 1 follows immediately. In practice interactions hybridize the discrete mode with higher configurations: part of the weight in $S(q, \omega)$ is an incoherent continuum and the discrete excitation energy ω_q is corrected, as described in the subsequent paper of Feynman and Cohen[3].

In order to put flesh on these handwaving ideas, we must treat the superfluid liquid and the solid in a common language. That is relatively easy for a lattice gas in which the length scale is put by hand, and where strong local correlations appear as constraints on the local Hilbert space. In section 2 we

clarify the interplay of superfluidity and Mott localization for a gas with one atom per site, $N = N_L$, with maximum occupancy $n_{\max} = 2$. That model is a simplified version of the general mean field picture of the Bangalore group [4]. A second order Mott transition occurs at a critical repulsion U^* , *where the superfluid order parameter vanishes continuously*. The excitation spectrum has a Goldstone mode at $q = 0$ as expected, but nothing happens at zone edge. Note that localization, characteristic of a solid, does not require a CDW, a point which has been emphasized by Anderson[5]

Breaking of translational symmetry by a CDW is introduced in section 3 within the pioneering model of Matsubara and Matsuda[6]: the band is half filled, $N = N_L/2$, and $n_{\max} = 2$. Such a hard core gas is isomorphous to a spin 1/2 problem. The hopping kinetic energy is a transverse ferromagnetic coupling that favours superfluidity (the azimuth of magnetization is the locked phase of the superfluid order parameter), for a half filled band a repulsion between nearest neighbour sites favours a CDW. Despite its half century of age that model has no wrinkles: a mean field approximation describes the superfluid-solid transition with amazing success. Near the transition the excitation spectrum displays the Goldstone mode at $q = 0$, as well as a soft mode at zone edge, which appears explicitly in the original paper, but which did not receive much attention. That model teaches us a lesson: *a superfluid close to a CDW instability has a dip in its excitation spectrum near the incipient Bragg spot*.

Lattice models have the virtue of simplicity, but they have one major drawback: the lattice is put by hand. Rotational symmetry is lost from the start, even the liquid is anisotropic: the physics behind a first order transition is lost. One would like an "isotropic theory of localization". In section 4 we propose a crude minimal formulation that meets that goal. It uses an expansion in powers of the condensate fraction N_o for a normal system whose soft density fluctuations are put by hand. We do not try to describe the CDW from scratch, we try instead to understand "delocalization via superfluidity". Our limit of small N_o is complementary to ordinary perturbation theory that starts from $N_o = N$. It is in no way "a" theory of ${}^4\text{He}$: the aim is a qualitative understanding of interplay between density fluctuations and superfluidity. We show that the CDW minimum ω_m in the normal density fluctuation spectrum carries over to the superfluid quasiparticles as a roton minimum, as expected. Moreover quantum fluctuations act to decrease even more our originally small N_o . In a lattice gas the soft mode occurred only at a single $q = G$ and the integrated quantum fluctuations remained minor

in 3 dimensions. In our isotropic system the soft mode extends over a whole sphere and quantum fluctuations become dramatically large. The smaller ω_m , the larger the depletion! We will show that the maximum value of N_o is of order ω_m^2 . The same CDW dip in charge excitations is thus responsible for (i) the roton minimum, (ii) the smallness of N_o .

Before that limit is reached, a first order transition should occur, which breaks rotational symmetry. Starting from a spherical soft mode, 4 tetrahedral feet should grow and "reach the ground", producing the Bragg spots of a BCC lattice. Because the CDW order parameter has no symmetry constraint, cubic terms in the Landau expansion do exist: the transition is definitely first order. These issues are briefly mentioned in the concluding section 5, but we make no attempt at formalizing them.

2 Superfluidity *vs* Mott localization

We consider a Hubbard Bose system on a lattice with nearest neighbour hopping: the hamiltonian may be written as

$$H = -tb_i^*b_j + \frac{U}{2}n_i(n_i - 1) + \epsilon n_i$$

The bandwidth is $2Zt$, where Z is the number of neighbours. For any integer filling, $N = pN_L$, a Mott localization transition should occur for strong enough repulsion U . Charge fluctuations acquire a gap, long range phase coherence is destroyed and superfluidity gives way to localization. A beautiful mean field formulation of the problem was given by the Bangalore group[4]. In order to emphasize the underlying physics we simplify the problem even further. We consider the case $N = N_L$ and we assume that the maximum occupancy at each site is $n_{\max} = 2$, the minimal non trivial problem: each site has three states $n_i = 0, 1, 2$. Due to Bose commutation rules the problem is exactly isomorphous to a spin 1 problem. S_{iz} is the local occupancy ($n_i - 1$), the spin raising operator $S_{i+} = (S_{ix} + iS_{iy}) / \sqrt{2}$ is the boson creation operator b_i^* , the hopping kinetic energy is a nearest neighbour ferromagnetic exchange, $-tS_{i+}S_{j-}$. We choose ϵ such that the $n_i = 0$ and 2 states are degenerate (particle hole symmetry). The local energy that lowers the $n_i = 1$ state is equivalent to an anisotropy energy $US_{iz}^2/2$ in the magnetic problem. The

resulting hamiltonian is

$$H = \sum_i \frac{U}{2} S_{iz}^2 - \frac{t}{2} \sum_{ij} [S_{ix}S_{jx} + S_{iy}S_{jy}]$$

Within a mean field approximation each site has the same spin state corresponding to $\overline{S_z} = 0$. The most general spin 1 state is characterized by a polarization, from linear through elliptic to circular, and by 3 Euler angles that fix the orientation of the ellipse (think of light!). A state $m = 0$ in any direction of quantization is linearly polarized along that direction, a state $m = 1$ is circularly polarized in the perpendicular plane. If U wins, the ground state is an anisotropy singlet $S_z = 0$: *localization corresponds to linear polarization*. If t wins, *circular polarization corresponding to superfluidity* holds with an axis in an arbitrary direction of the (x, y) plane - say the x axis, $\overline{S_{ix}} \neq 0$. Since an elliptic state is a superposition of two linear polarizations along z and y in quadrature we can go smoothly from localization to superfluidity playing with ellipticity: we have all the ingredients of a second order Mott transition.

Let us quantize spins along the z axis. The above interpolation corresponds to a state

$$\begin{bmatrix} \frac{\sin \theta}{\sqrt{2}} \\ \cos \theta \\ \frac{\sin \theta}{\sqrt{2}} \end{bmatrix}$$

Simple algebra yields the expectation value $\overline{S_x} = \sin 2\theta$ and the resulting mean field energy per site

$$E_o = \frac{U}{2} \sin^2 \theta - \frac{1}{2} Zt \sin^2 2\theta$$

which should be minimized with respect to θ . For strong repulsion $U > 4Zt$ the minimum is achieved at $\theta = 0$: the ground state is a Mott insulator with a frozen filling $n_i = 1$. In the opposite case $U < 4Zt$ the minimum θ^* corresponds to

$$\cos 2\theta^* = \frac{U}{4Zt} \tag{2}$$

A non interacting gas corresponds to $\theta^* = \pi/4$, *i.e.* to circular polarization $\overline{S_x} = 1$. As surmised the transition at $U = 4Zt$ is continuous, with a vanishing superfluid order parameter $\overline{b_i^*} = \overline{S_x}/\sqrt{2}$. This is the central result of [4]: *Mott*

localization reduces the superfluid order parameter ("condensate fraction") to 0 at the transition".

That same mean field approach yields the elementary excitation spectrum. Usually one writes equations of motion for the creation operator X_q^*

$$[H, X_q^*] = \omega_q X_q^*$$

Such a method works, but it is clumsy as it generates an army of operators which in turn request equations of motion. It is much simpler to study small amplitude deformations of the wave function using the Schrödinger equation. That less usual technique is sketched in Appendix 1: here we only quote results in order to stress their evolution. The excitation spectrum has two branches. One is the standard spin wave generated by rotations S_{iz} and S_{iy} , corresponding to a perturbation

$$|\psi_{i1}\rangle = \begin{bmatrix} \alpha_i(t) \\ 0 \\ -\alpha_i(t) \end{bmatrix}$$

Such a mode combines rotation and ellipticity in the (x, z) plane. The resulting spectrum is

$$\begin{aligned} \omega_q^2 &= K(K - 2ZJ\gamma_q) && \text{in the localized state } K > 2ZJ \\ \omega_q^2 &= [2ZJ \cos^2 \theta]^2 (1 - \gamma_q) && \text{in the superfluid state } K < 2ZJ \end{aligned} \quad (3)$$

in which γ_q is the usual phase shift factor

$$\gamma_q = \frac{1}{Z} \sum_{\delta} \exp(iq\delta)$$

In the localized state ω_q has a gap. In the superfluid we recover the familiar gapless Goldstone mode, with a linear spectrum that corresponds to phonons in the Bose liquid. Note the continuity.

The other branch describes modulation of ellipticity in the (y, z) plane. It corresponds to an even perturbation

$$|\psi_{i1}\rangle = \begin{bmatrix} \alpha_i(t) \\ 0 \\ \alpha_i(t) \end{bmatrix}$$

which must be orthogonalized to the ground state. It is a "hard mode" which affects the structure of the state. In the localized state we recover the same spectrum $\omega_q^2 = K(K - 2ZJ\gamma_q)$, as expected since the singlet $S_z = 0$ does not make any difference between (x, z) and (y, z) planes. That rotational symmetry is lost in the superfluid for which we find

$$\omega^2 = (2ZJ)^2 [1 - \gamma_q \cos^2 2\theta] \quad (4)$$

A gap persists at zone center, as expected. Everything is continuous at the transition, with the appropriate symmetries. These two branches are sketched on Fig.1: *the important fact is the lack of any soft mode at zone edge*. In this model localization is "pure", implying no breakdown of translational symmetry (the lattice cell remains the one put by hand at the beginning). Nothing should happen at zone edge - and nothing does!

3 Superfluidity *vs* charge density wave

Localization can also occur for fractional filling if we allow for breaking of translational symmetry, via a charge density wave. The latter increases the unit cell, thereby changing the physics. Let us consider a half filled band in a nested lattice, $N = N_L/2$. The simplest non trivial model is a hard core gas, in which only the local occupancies $n_i = 0, 1$ are allowed. Such a problem is isomorphous to a spin 1/2 system, just as the three state problem was isomorphous to spin 1. The raising operator $S_{i+} = S_{ix} + iS_{iy}$ is the boson creation operator b_i^* and the hopping kinetic energy is a transverse ferromagnetic coupling: once more the azimuth of S is the gauge phase. If there is no interaction beyond the hard core nothing can oppose hopping and the ground state is superfluid. In order to favour a charge density wave (*i.e.* the solid phase), we must add a nearest neighbour repulsion $Vn_in_j/2$ that pushes particles apart. We thus write the Hamiltonian as

$$H = - \sum_{i,j} t (S_{ix}S_{jx} + S_{iy}S_{jy}) + \frac{V}{2} S_{iz}S_{jz}$$

If V wins, the ground state for half filling is an Ising antiferromagnet, with one filled sublattice $S_z = +1/2$, the other one $S_z = -1/2$ being empty: the liquid has crystallized! Such an Hamiltonian was introduced nearly 50 years ago in a pioneering paper of Matsubara and Matsuda [6], precisely in

order to describe the superfluid-solid transition of ${}^4\text{He}$. They treat it within a mean field approximation, allowing for simultaneous breaking of gauge and translational symmetries (the so called supersolid). All spins have the same component $S_x = \cos \theta$, and alternating components $S_z = \pm \sin \theta$. The corresponding ground state energy is

$$E_o = -NZ \left[t \cos^2 \theta + \frac{V}{2} \sin^2 \theta \right]$$

Hence two possibilities:

- if $V < 2t$ the angle $\theta = 0$ and the ground state is superfluid,
- if $V > 2t$ the angle $\theta = \pi/2$ and the ground state is a CDW crystal.

In this model the transition is first order and the intermediate supersolid never occurs. If one adds a second neighbour interaction one may either favour the supersolid or reinforce the first order transition. There is a vast literature on the subject which we ignore: we stick to the most naive model

While the losing order parameter disappears in the mean field ground state, it should manifest itself as a soft mode in the excitation spectrum. Think for instance of a paramagnet close to antiferromagnetism: a soft zone edge spin wave signals the proximity of the transition. The same is true here: a superfluid close to crystallization should show up a soft CDW mode at zone edge. Indeed we can write the standard equations of motion starting from the pure superfluid state $\overline{S_{ix}} = 1/2$

$$\begin{aligned} \frac{dS_{iz}}{dt} &= -it [S_{iy}S_{jx} - S_{ix}S_{jy}] = -\frac{iZt}{2} (1 - \gamma_q) S_{iy} \\ \frac{dS_{iy}}{dt} &= +itS_{iz}S_{jx} + \frac{iV}{2} S_{ix}S_{jz} = \frac{iZ}{2} \left(t + \frac{V}{2}\gamma_q \right) \end{aligned}$$

(We use the same notations as in the preceding section). Altogether we find a dispersion relation

$$\omega^2 = \frac{Z^2}{4} t (1 - \gamma_q) \left(t + \frac{V}{2}\gamma_q \right) \quad (5)$$

Because $(1 - \gamma_q)$ behaves as q^2 near $q = 0$ a linear spectrum ensues at long wave length, corresponding to the phonon branch of liquid ${}^4\text{He}$. That was a major achievement of Matsubara and Matsuda [6] (the usual q^2 spectrum of a ferromagnet becomes linear because the z part of exchange is missing). But that result has another equally interesting feature at zone edge $\gamma_q = -1$:

the frequency $\omega^2 = \frac{tZ^2}{4} (2t - V)$ vanishes at the transition! The soft CDW mode we are looking for is there, as shown in Fig. 2. Strangely enough that result is not emphasized in the 1956 paper.

That brief discussion teaches us one more lesson: *any localization transition that involves breaking of translational symmetry generates a soft mode that vanishes at the transition.* The resemblance with a roton minimum is striking. Because the transition is here first order the other salient feature, namely the vanishing of the superfluid order parameter at localization, is not present. In presenting these two naive models our aim was to show that these two features are distinct despite the fact they go hand in hand. A soft mode requires CDW symmetry breaking, while a small condensate does not. But both are signals of a pending crystallization.

4 An attempt at real liquids

Lattice models have the virtue of simplicity and elegance - but they are not fully convincing as the lattice is put by hand. Rotational symmetry of the liquid is lost from the very beginning. As a result soft density modes appear at points in the Brillouin zone (the zone edge), while in a regular liquid they should spread over a sphere with radius q_m . Of course first order freezing will generate discrete Bragg spots, but before it occurs fluctuations are isotropic. That is not a point of semantics: a sphere of soft modes is a little bit like a 1d system, with greatly enhanced quantum fluctuations (the "soft phase space" spreads over an area $4\pi q_m^2$). Since in the end quantum fluctuations are responsible for depleting the condensate, one may fear that lattice models grossly distort reality. In this section we propose a very crude argument that might circumvent these difficulties, at least qualitatively. The main idea is to start from the normal limit $N_o = 0$ instead of the free gas as usually done in perturbative approaches.

A central feature of superfluid Bose liquids is the hybridization of density fluctuations, described by particle hole pairs $b_{k+q}^* b_k$, with single particle excitations, describing creation b_q^* or destruction b_{-q} of a particle. Put another way the single particle Green's function $G(q, \omega)$ is linearly coupled to the charge response function $\chi(q, \omega)$. Both have the same eigenmodes, but with different weights. The coupling is due to "three leg vertices" sketched on Fig. 3a, where the dotted line represents a condensate operator, replaced by a c-number $\sqrt{N_o}$.

Assume first that there is no condensate, $N_o = 0$: the charge response function $\chi_n(q, \omega)$ is that of a "normal" liquid, carrying information on the dynamics of density fluctuations. If we had a solid it would correspond to a phonon spectrum. Here it is certainly more complicated, since anharmonicities couple a single phonon to higher configurations. We will nevertheless mimic χ_n by a single mode approximation, a simplification which looks sensible for a Bose liquid (it does hold at low energy for the superfluid). Let Ω_q be that energy, which is our basic phenomenological ingredient. In a translationally invariant system $\chi_n(q, \omega)$ obeys the f-sum rule: the full density response function follows at once

$$\chi_n(q, \omega) = \frac{Nq^2/m}{\Omega_q^2 - \omega^2} \quad (6)$$

All the physics lies in Ω_q . If we approach a CDW instability we expect Ω_q to display a soft mode with a minimum Ω_m at $q = q_m$. As long as the crystal is not frozen that minimum remains isotropic (corresponding to local crystalline order with fluctuating orientation). We do not attempt a microscopic calculation of Ω_q , which would be very difficult. We take it instead as the input of our estimate. We view that soft mode as the crucial feature of the problem, and we retain only those terms which are directly sensitive to it.

If there is no condensate the single particle Green's function $G_n(q, \omega)$ is not directly coupled to density fluctuations. It can be expressed as usual in terms of a self energy $\Sigma_n(q, \omega)$

$$G_n(q, \omega) = \frac{1}{\omega + \mu - q^2/2m - \Sigma_n(q, \omega)}$$

where μ is the chemical potential. We also mimic it by a single mode approximation, writing

$$G_n(q, \omega) = \frac{1}{\omega - \xi_q} \quad (7)$$

(the chemical potential is absorbed in the definition of ξ_q). We have no justification for that except convenience for further algebra. A more realistic G_n will not affect our qualitative conclusions much, and transparency is worth a few oversimplifications! For intermediate coupling ξ_q is comparable to the kinetic energy $\hbar^2 q^2/2m$ or to the interaction energy NU . Whether ξ_q vanishes at $q = 0$ in the "normal state" is not clear at this stage - see below. We now establish a small condensate fraction N_o : as shown in the famous

paper of Beliaev[8] condensate coherence leads to "anomalous" propagators $\widehat{G}(q, \omega) = \langle b_q b_{-q} \rangle$ (as in a superconductor) and to a corresponding self energy $\widehat{\Sigma}(q, \omega)$. The Dyson equation becomes a 2×2 matrix, the solution of which is particularly simple if we assume that Σ and $\widehat{\Sigma}$ are even functions of ω , a behaviour which will turn out to hold in our approximation:

$$G(q, \omega) = \frac{\xi_q + \omega + \Sigma}{\omega^2 - (\xi_q + \Sigma)^2 - \widehat{\Sigma}^2}$$

The energies of elementary excitations are the poles of G .

Leading contributions to Σ and $\widehat{\Sigma}$ contain 2 condensate lines, which can be anywhere inside the selfenergy diagram. Besides the first order Fock term of Fig. 3b,c, the only diagrams that couple directly (linearly) to the density soft mode are those of Fig. 3d,e. Sticking to our philosophy we thus write

$$\Sigma(q, \omega) = \widehat{\Sigma}(q, \omega) = n_o [U - U^2 \chi_n(q, \omega)] \quad (8)$$

Note that χ_n is an even function of ω which justifies our previous statement. These selfenergies are responsible for hybridization of G and χ_n . In this crude approximation $\Sigma = \widehat{\Sigma}$: the secular equation for quasiparticles is simply

$$\omega^2 = \xi_q^2 + 2\xi_q \Sigma \quad (9)$$

This is to be compared to the so called Hugenholtz-Pines theorem [7] (which guarantees a gapless spectrum of the superfluid at $T = 0$)

$$\Sigma - \widehat{\Sigma} - \mu = 0 \quad \text{at } q = \omega = 0$$

It follows that the energy ξ_q that parametrizes G_n vanishes at $q = 0$.

If we retain only the Fock term in Σ we obtain the familiar Bogoliubov spectrum

$$\omega = \varepsilon_q^B = [\xi_q^2 + 2\xi_q N_o U]^{1/2} \quad (10)$$

Adding hybridization to density fluctuations transforms 10 into

$$\omega^2 = \varepsilon_q^{B2} - \frac{N_o}{N} \cdot \frac{\Lambda_q}{\Omega_q^2 - \omega^2} \quad (11)$$

in which we have set

$$\Lambda_q = 2\xi_q \frac{q^2}{m} (NU)^2 \quad (12)$$

For intermediate coupling, all energies inside Λ_q are comparable in the roton region: Λ_q is of order ξ_q^4 . We see that hybridization to density fluctuations is proportional to N_o/N , as expected. The problem that emerges is *anticrossing of two modes*, ε_q^B and Ω_q , linearly coupled by $\Lambda_q N_o/N$, as sketched in Fig.4. The physics behind that result is quite clear: one can consider the density mode Ω_q as an independent "phonon" degree freedom. The effective interaction between bosons has a direct repulsion U , and a phonon mediated attraction, as in the standard Bardeen picture of electron phonon interaction. The two terms of Σ correspond to these two interactions. While for fermions phonons couple to a continuum, here they couple to a single mode - hence the hybridization picture.

Let us first look at the excitation spectrum near the minimum Ω_m . We assume that the minimum is deep, $\Omega_q \ll \varepsilon_q^B$. The lower mode $\omega = E_{q-}$ corresponds to

$$E_{q-}^2 \approx \Omega_q^2 - \frac{N_o}{N} \cdot \frac{\Lambda_q}{\varepsilon_q^{B2}}$$

The condensate lowers the roton minimum. If N_o is too large the frequency ω becomes pure imaginary: the density fluctuation turns unstable and crystallization of the CDW ensues. That instability puts an upper bound on N_o

$$\frac{N_o^{\max}}{N} = \frac{\Omega_q^2 \varepsilon_q^{B2}}{\Lambda_q} \approx \frac{\Omega_q^2}{\xi_q^2} \quad (13)$$

That boundary is small: *a soft CDW mode implies a small condensate population*, as found in superfluid ^4He . But nevertheless the normal state is always unstable to superfluidity: an infinitesimal N_o lowers the ground state energy. The latter is just the zero point energy of all the eigenmodes

$$U_o = \frac{1}{2} \sum_q (E_{q-} + E_{q+})$$

where - and + refer to the lower and upper modes. The secular equation being biquadratic, E_{q-}^2 and E_{q+}^2 move by opposite amounts - hence E_{q-} moves down more than E_{q+} moves up: U_o is lowered by the condensate. *Superfluidity always appears as long as crystallization is not frozen, as foreseen in our lattice models.* The crucial question is then why does N_o saturate?

A possible answer is the effect of depletion. It is well known that quantum fluctuations promote condensate bosons into finite momentum states, thereby decreasing N_o . If that depletion is larger than the small N_o we start from, a

condensate cannot survive. We propose that such a threshold is reached when the renormalized roton minimum E_m is small enough. Since E_m is monitored by N_o , that puts an upper limit to the condensate population which is lower than the bifurcation limit N_o^{\max} . It is clear that such an iterative argument is very crude: a real calculation of N_o should be self consistent! That implies including quantum fluctuations in the theory from the very beginning, which is a formidable task. Here we calculate quantum fluctuations with the bare N_o instead of the final one. Our hope is that such a naive approach will convey the qualitative physics (N_o is bound by quantum fluctuations) and yield the correct orders of magnitude. Anyhow, we have made so many wild simplifications that we should stick to our philosophy!

What we need is an extension of the standard Bogoliubov algebra to the case of two coupled excitations. Because the real modes are mixtures of bosons and phonons, such an extension requires care. Let us represent the normal state density response function $\chi_n(q, \omega)$ in terms of phonons characterized by creation operators a_q^* . We write the Hamiltonian as

$$\begin{aligned} H &= \sum_q \left[\xi_q b_q^* b_q + \frac{N_o U}{2} (b_q^* + b_{-q}) (b_q + b_{-q}^*) + \Omega_q a_q^* a_q \right] + H_{hyb} \quad (14) \\ H_{hyb} &= \sum_q \left[\alpha_q (b_q^* + b_{-q}) (a_q + a_{-q}^*) \right] \end{aligned}$$

That hamiltonian is bilinear and therefore it can be diagonalized exactly. In order to establish its equivalence with our former problem we look for elementary excitations with creation operator β_q^* of the form

$$\beta_q^* = u_q b_q^* + v_q b_{-q} + w_q a_q^* + x_q a_{-q} \quad (15)$$

that should obey the equation of motion

$$[H, \beta_q^*] = E_q \beta_q^* \quad (16)$$

The algebra is straightforward, yielding the set of equations

$$\begin{aligned} (E_q - \xi_q) u_q &= (E_q + \xi_q) v_q = N_o U (u_q - v_q) + \alpha_q (w_q - x_q) \quad (17) \\ (E_q - \Omega_q) w_q &= (E_q + \Omega_q) x_q = \alpha_q (u_q - v_q) \end{aligned}$$

from which we infer

$$(w_q - x_q) = (u_q - v_q) \frac{2\Omega_q \alpha_q}{E_q^2 - \Omega_q^2}$$

From the first equation 17 we obtain

$$\begin{aligned} u_q &= \frac{\Sigma}{E_q - \xi_q} (u_q - v_q) \quad , \quad v_q = \frac{\Sigma}{E_q + \xi_q} (u_q - v_q) \\ \Sigma &= N_o U - \frac{2\Omega_q \alpha_q^2}{\Omega_q^2 - E_q^2} \end{aligned} \quad (18)$$

Subtracting the first two equations 18 we obtain the dispersion equation

$$1 = \Sigma \left[\frac{1}{E_q - \xi_q} - \frac{1}{E_q + \xi_q} \right] = \frac{2\xi_q \Sigma}{E_q^2 - \xi_q^2}$$

which is identical to 11 and 12 if we choose

$$\alpha_q = \sqrt{\frac{N_o N U^2 q^2}{2m\Omega_q}} \quad (19)$$

Note that α_q has the dimension of an energy, which is large, $\approx \xi_q \sqrt{\xi_q/\Omega_q}$. For each q there exist two modes, with coefficients u_q^\pm , etc... Equations 17 determine these coefficients within an arbitrary factor: we normalize them in such a way as to fulfill the commutation rule $[\beta_q, \beta_q^*] = 1$, which implies

$$|u_q|^2 - |v_q|^2 + |w_q|^2 - |x_q|^2 = 1 \quad (20)$$

Elementary excitations are thus well specified.

The ground state is the vacuum of quasiparticles: in order to obtain depletion we must invert the Bogoliubov transformation and express b_q^* in the form

$$b_q^* = \sum_i \left(r_q^i \beta_q^{i*} + s_q^i \beta_{-q}^i \right)$$

where $i = \pm$ refers to the two modes. The zero temperature condensate depletion due to the states $(q, -q)$ is equal to

$$n_q = \overline{b_q^* b_q} = |s_q^-|^2 + |s_q^+|^2 \quad (21)$$

We just need to invert a 4×4 matrix. The calculation is easy if we exploit the smallness of N_o (we identify the leading coefficient and we scale the other ones with respect to it). The algebra is sketched in Appendix 2. We find that s_q^+ is negligible, while

$$s_q^- = \frac{\alpha_q}{\xi_q} \sqrt{\frac{\Omega_q}{E_q}}$$

Replacing α_q by its value 19 we obtain the depletion n_q

$$n_q = \frac{NN_oU^2q^2}{2m\xi_q^2E_q} = \frac{N_o}{N} \cdot \frac{\Lambda_q}{4\xi_q^3E_q} \quad (22)$$

where Λ_q has been defined in 12. Note that depletion is of order N_o : it directly competes with the condensate population we started from.

Ignoring self consistency, superfluidity is only possible if

$$\sum_q n_q < N_o$$

which implies

$$\sum_q \frac{\Lambda_q}{4\xi_q^3E_q} < N \quad (23)$$

In practice the summation is controlled by the roton minimum

$$E_q = E_m + \gamma(q - q_m)^2$$

The condition 23 may be written as

$$\frac{4\pi q_m^2}{8\pi^3} \cdot \frac{\Lambda_m}{4\xi_m^3} \cdot \frac{\pi}{\sqrt{E_m\gamma}} < N \quad (24)$$

Since the CDW creates a lattice with one atom per site, we must have

$$N = \frac{q_m^3}{6\pi^2} \cdot \eta$$

where $\eta \sim 1$. In order to achieve superfluidity the roton minimum must obey the condition

$$\frac{3\pi}{4} \frac{\Lambda_m}{\xi_m^3 \sqrt{E_m\gamma} q_m^2} < \eta \quad (25)$$

The roton minimum cannot be too shallow, unless it is very narrow.

Assume first that N_o is infinitesimal: the minimum E_m is the bare Ω_m , which must obey 25. If N_o grows, E_m decreases. If the saturation mechanism for N_o is indeed depletion, the inequality in 25 must become a near equality (a crude order of magnitude estimate since a real calculation should be self consistent). Roughly speaking the observed spectrum should be such that

$$\frac{3\pi}{4} \frac{\Lambda_m}{\xi_m^3 \sqrt{E_m\gamma} q_m^2} \sim 1 \quad (26)$$

The value of N_o then depends on the difference between the final E_m and the bare Ω_m

$$\frac{N_o}{N} = (\Omega_m^2 - E_m^2) \frac{\varepsilon_{qB}^2}{\Lambda_q} \quad (27)$$

As expected, N_o is small!

Our argument is admittedly extremely crude. It suggests one qualitative fact: *a roton minimum signalling the approach to cristallization destroys superfluidity before the renormalized E_m goes to zero.*

5 Conclusion

The main purpose of this article is to look at superfluid ${}^4\text{He}$ from an unusual vantage point, starting from the solid rather than from the dilute gas as usual. We assume that the density response function has a soft CDW mode signalling the proximity of crystallization, which has nothing to do with Bose Einstein condensation, and we we look at the effect of superfluidity, characterized by a *small* condensate population N_o . Energywise the condensate is always favourable as long as it does not trigger the CDW instability: the latter constraint puts an upper limit on N_o which is small if the roton minimum is shallow. More subtle, depletion due to quantum fluctuations should not exceed the small value of N_o we started from. Due to that effect we find that *superfluidity disappears before vanishing of the renormalized roton minimum E_m* . If crystallization were a second order transition, there should exist a region where the ground state is a "normal liquid", whatever it is. In practice crystallization is a first order transition and the above statement does not contradict facts. Of course this conclusion holds only for small N_o : it is irrelevant in the opposite Bogoliubov limit. If the saturation of N_o relies on depletion, we find a relation between the renormalized E_m and the roton effective mass (curvature of Ω_q). Our approach being only qualitative, that relation cannot be compared to experiments, but it yields orders of magnitude. Once E_m is known the condensate fraction N_o is determined by the difference between E_m and the original roton minimum Ω_m (in the absence of superfluidity): *it is small for low energy rotons*. We emphasize that this is *in no way* a theory of liquid ${}^4\text{He}$: a manageable algebra implies staying a long distance away from reality! But we believe that the present model is qualitatively closer to real helium than the Bogoliubov calculation.

We have been concerned only with the liquid before it crystallizes: the system retains full isotropy. In practice the CDW instability selects a few discrete points out of the sphere of soft modes, that freeze and provide the Bragg spots of the crystal. That selection breaks rotational invariance, as befits a lattice geometry (the frozen modes stabilize the other ones). Let G_1, G_2, G_3 be the Bragg vectors, ρ_1, ρ_2, ρ_3 the corresponding Fourier components of the density. Within a mean field approach one might write a Landau energy

$$U = A \sum_i \rho_i^2 + \sum_{ij} B_{ij} \rho_i^2 \rho_j^2$$

If the signature of B_{ij} is positive the transition is second order, if it is negative it is first order. Here that conclusion is wrong because of possible cubic terms. In usual problems such as magnetism the symmetry upon reversal of magnetization precludes such terms. Here we deal with density, for which such a symmetry does not hold. The only feature that remains is translational invariance: a cubic term $\rho_1 \rho_2 \rho_3$ can exist only if $G_1 + G_2 + G_3 = 0$. If all G_i have the same modulus (they arise from the sphere of soft modes), they must form an equilateral triangle. Once they exist, the cubic terms necessarily produce a first order transition before the threshold $E_m = 0$ is reached. In 2D that corresponds to an hexagonal lattice. In 3D the reciprocal lattice must be FCC (the first Bragg spots form a tetrahedron), implying a BCC direct lattice. That holds as long as $E_m > 0$. Once $E_m < 0$ the quartic terms quickly take over and they can favour any type of lattice. The geometry of crystallization is a very general issue that extends far beyond liquid helium. We mention it only as a word of care. For more details, see for instance [9]

Acknowledgements

The similarities between liquid and solid helium were stressed around 1980 by Albert Libchaber, then in Paris: he challenged me to find an explanation: this paper is a belated reply! I am grateful to Antoine Georges for drawing my attention again to that question. I benefited from many discussions with Efim Kats: his critical look was very helpful. Finally I want to present this work to David Pines on the occasion of his 80th birthday. He guided my first steps in many body physics nearly 50 years ago: he knows how grateful I am to him. He likes somewhat heretical views: this is one which he may well destroy!

A Appendix 1

Elementary excitations are usually found via an operator equation for their creation operator X^*

$$[H, X^*] = EX^*$$

Such a method is fine as long as the commutator generates operators that belong to the same manifold one started from. Our spin 1 problem provides a counterexample which generates an army of new operators at each commutation. Sure it will eventually stop and the method can be brought to completion! But one can short circuit the complications working with the wave function instead of operators. This appendix shows how to proceed. We start from the ground state $|\Psi_o\rangle$ and we treat a small admixture $|\Psi_1(t)\rangle$ up to *first order*. $|\Psi_1\rangle$ is kept orthogonal to $|\Psi_o\rangle$ so that it does not affect normalization. Within a mean field approximation we consider the dynamics of a given site. The perturbation modifies the effective field created by neighbouring sites: the local hamiltonian therefore contains the zeroth order mean field contribution H_o and a time dependent correction H_1 which is a statistical average of the neighbours modulation. The first order single site Schrödinger equation reads

$$i\frac{\partial |\Psi_1\rangle}{\partial t} = (H_o - e_o) |\Psi_1\rangle + H_1 |\Psi_o\rangle$$

We have subtracted from H_o the local ground state energy e_o (*without the factor 1/2 for interactions*), in such a way as to maintain orthogonalization. (Put another way the excited state dynamics must be measured with respect to the ground state precession). An elementary excitation with energy E corresponds to a perturbation such that

$$i\frac{\partial |\Psi_1\rangle}{\partial t} = E |\Psi_1\rangle$$

There are far less states than operators - hence a much more compact formulation.

We illustrate our point on our spin 1 problem. The local ground state $|\Psi_o\rangle$ is

$$\begin{bmatrix} \sin \theta / \sqrt{2} \\ \cos \theta \\ \sin \theta / \sqrt{2} \end{bmatrix}$$

There exist only two orthogonal perturbations

$$\begin{bmatrix} \alpha \\ 0 \\ -\alpha \end{bmatrix}, \quad \begin{bmatrix} \alpha \cos \theta \\ -\alpha \sqrt{2} \sin \theta \\ \alpha \cos \theta \end{bmatrix}$$

The first one is a rotation generated by S_y and S_z : it corresponds to spin waves. The other one is a modulation of excentricity, sensitive to anisotropy. Let us consider first the odd spin wave mode. Neighbouring sites are sensed by the modulation of $\overline{S_{jz}}$ and $\overline{S_{jy}}$. Only the latter matters since the exchange has no Ising term,

$$\overline{S_{jy}} = i\sqrt{2} \cos \theta (\alpha_j - \alpha_j^*)$$

Treating the phase shift from site to site via the usual factor γ_q , we write the first order Schrödinger equation as

$$i \frac{\partial \alpha}{\partial t} = (K - e_o) \alpha - 2ZJ\gamma_q \cos^2 \theta (\alpha - \alpha^*)$$

Separating the real and imaginary parts we obtain the secular equation

$$\omega^2 = (K - e_o) (K - e_o - 2ZJ\gamma_q \cos^2 \theta)$$

We have seen that $e_o = K \sin^2 \theta - ZJ \sin^2 2\theta$, hence

$$\omega^2 = (K \cos^2 \theta + ZJ \sin^2 2\theta) (K \cos^2 \theta + ZJ\gamma_q [\sin^2 2\theta - 2\gamma_q \cos^2 \theta])$$

We thus recover in a few lines the results quoted in the text, both in the localized state $\theta = 0$ and in the superfluid $\cos 2\theta = K/2ZJ$.

A similar calculation holds for the even mode, for which the modulation affects S_x :

$$\overline{S_{jx}} = \sqrt{2} \cos \theta (\alpha_j + \alpha_j^*)$$

The calculation is similar, but for one complication in the superfluid state: $H_1 |\Psi_o\rangle$ does not respect the orthogonality constraint. One must project that term on the subspace orthogonal to $|\Psi_o\rangle$, which is equivalent to replacing S_x by $(S_x - \overline{S_x})$ in the time dependent local hamiltonian

$$-ZJ\gamma_q \overline{S_x} (S_x - \overline{S_x})$$

The Schrödinger equation for α reads (for the superfluid)

$$i \frac{\partial \alpha}{\partial t} = 2ZJ\alpha - ZJ\gamma_q \cos^2 \theta (\alpha + \alpha^*)$$

We recover in that way all the results quoted in the text. Using wave functions simplifies life!

B Appendix 2

In order to invert the Bogoliubov transformation we start from 17. For the upper mode the condensate is a small perturbation: the leading term in β_q^* is b_q^* , implying $u_q = 1$. The three other coefficients

$$v_q^+ = \frac{E_q - \xi_q}{E_q + \xi_q} \approx \frac{\Sigma}{2\xi_q} \sim \frac{N_o}{N}$$

$$w_q^+ \approx x_q^+ \approx \frac{\alpha_q}{\xi_q} \sim \sqrt{\frac{N_o}{N} \frac{\xi_q}{\Omega_q}}$$

For the lower mode, the dominant terms are w_q^- and x_q^- (quasiparticles are mostly phonons). They are normalized so that $w_q^{-2} - x_q^{-2} = 1$. Using 17 we find immediately

$$w_q^- = \frac{E_q + \Omega_q}{2\sqrt{E_q\Omega_q}}, \quad x_q^- = \frac{E_q - \Omega_q}{2\sqrt{E_q\Omega_q}}$$

from which we infer

$$v_q^- = -u_q^- = \frac{v_q^- - u_q^-}{2} = \frac{\Omega_q^2 - E_q^2}{4\alpha_q\sqrt{E_q\Omega_q}}$$

The 4×4 matrix that relates $\beta^{+*}, \beta^+, \beta^{-*}, \beta^-$ to b^*, b, a^*, a is thus

$$\begin{bmatrix} 1 & v_q^+ & \alpha_q/\xi_q & \alpha_q/\xi_q \\ v_q^+ & 1 & \alpha_q/\xi_q & \alpha_q/\xi_q \\ -v_q^- & v_q^- & w_q^- & x_q^- \\ v_q^- & -v_q^- & x_q^- & w_q^- \end{bmatrix}$$

The determinant of the matrix is 1 since we normalized the quasiparticles. The inverse matrix is obtained calculating minors. Let us first ignore v_q^+ . For the upper mode we erase the first column and the second line: the minor vanishes, implying $s_q^+ = 0$. For the lower mode we erase the first column and the fourth line: the minor is

$$\frac{\alpha_q}{\xi_q} (w_q - x_q) = \frac{\alpha_q}{\xi_q} \sqrt{\frac{\Omega_q}{E_q}}$$

which is the result quoted in the text. It is easily verified that the contribution of v_q^+ is negligible compared to that leading term.

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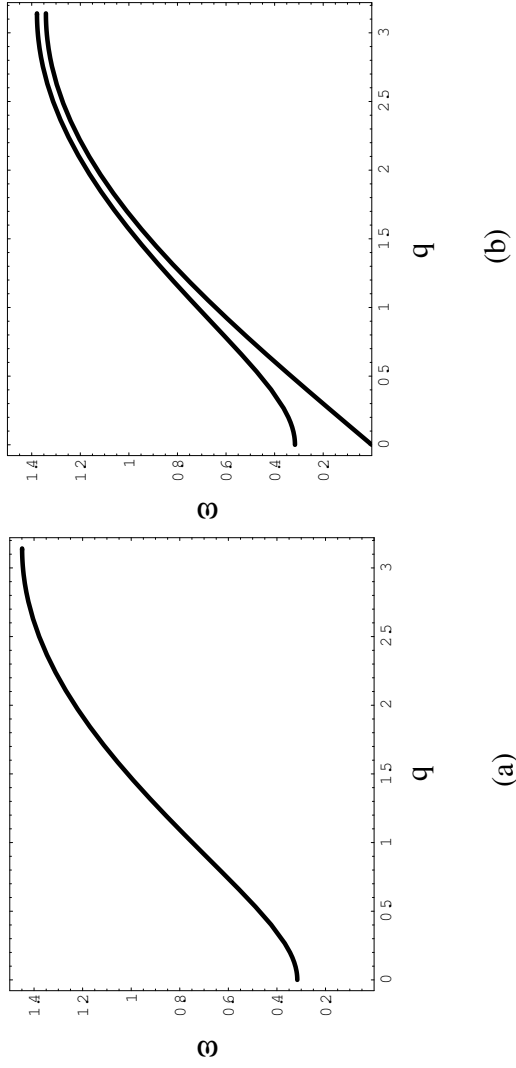


Figure 1: The elementary excitations of the insulator along the diagonal in the Brillouin zone [(a) $K/(2ZJ)=1.2$], and of the superfluid [(b) $K/(2ZJ) = 0.8$] in the filled band.

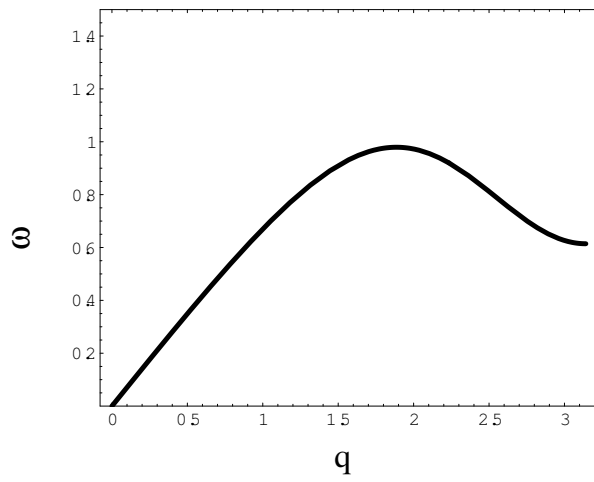


Figure 2: The elementary excitations of the superfluid phase along the diagonal of the Brillouin zone for half filled band near the localization transition.

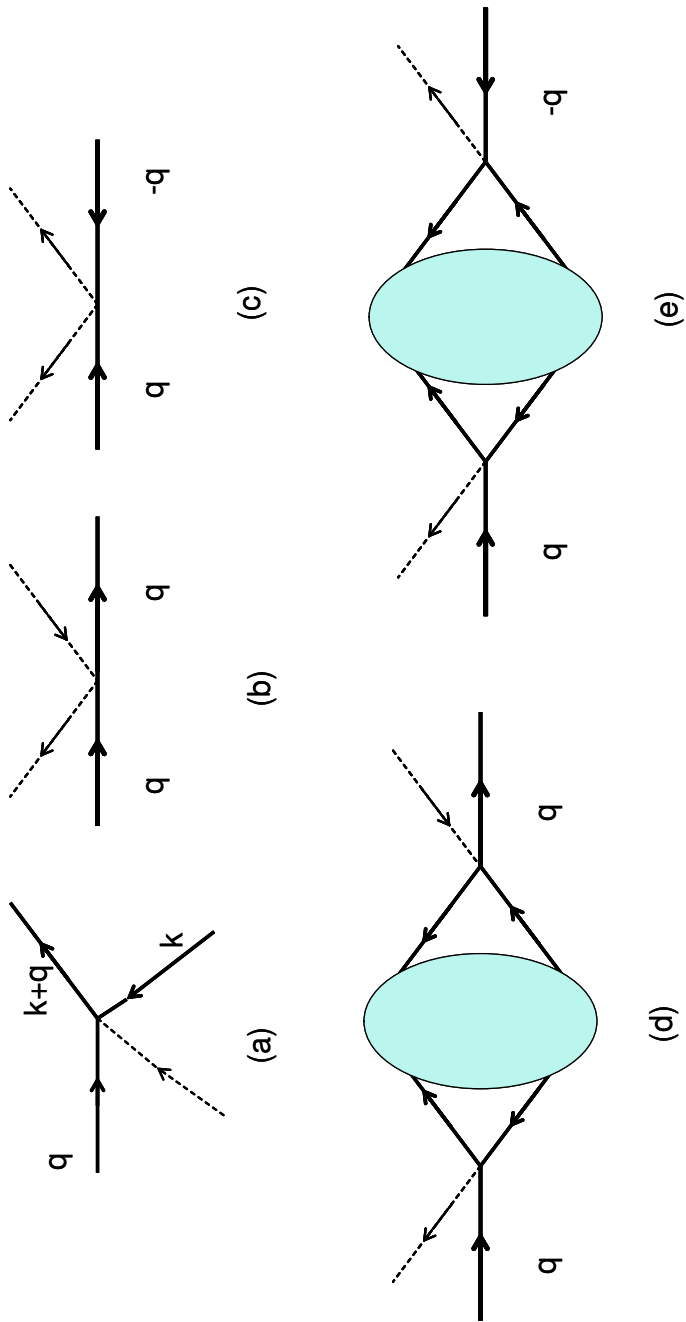


Figure 3: (a) the basic hybridization vertex. (b), (c) the Bogoliubov self energies. (d), (e), hybridization of the charge density fluctuations. Dotted lines correspond to the condensate.

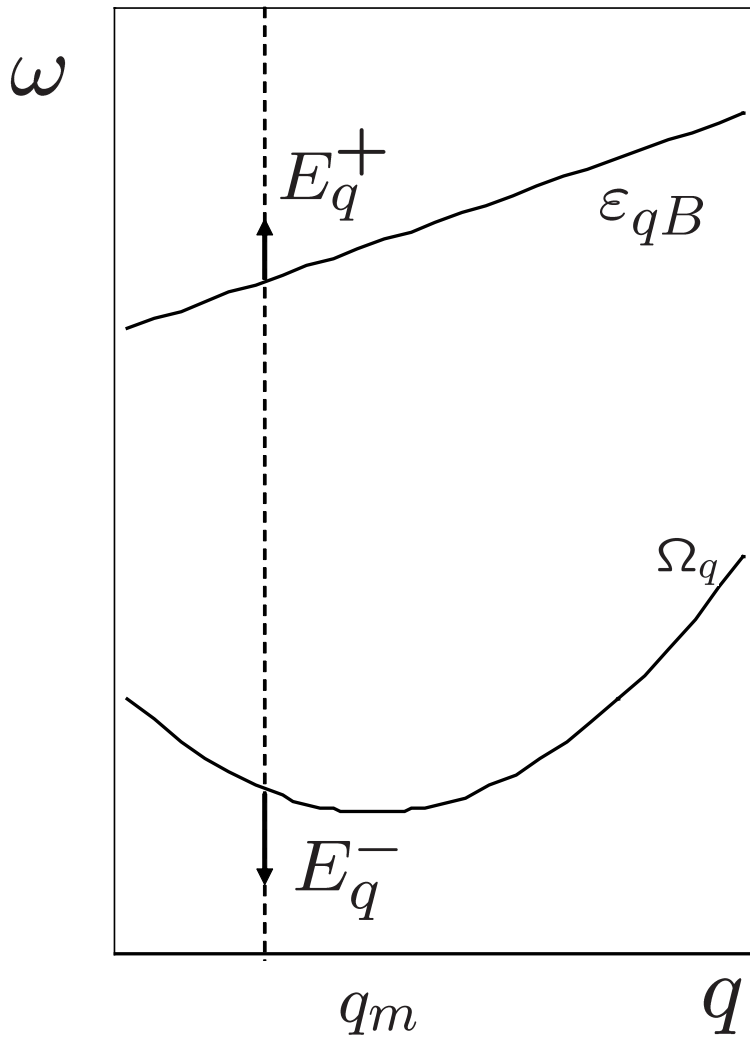


Figure 4: The basic hybridization mechanism: the Bogoliubov quasiparticle goes up and the charge density wave poles down.