## Triplet pairing in fermionic droplets

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We have investigated, in the L-S coupling, the appearance of triplet pairing in fermionic droplets in which a single nl shell is active. The method is applied to a constant-strength model, for which we discuss the different phase transitions that take place as the number of particles in the shell is varied. Drops of  $^3$ He atoms can be plausible physical scenarios for the realization of the model.

#### I. INTRODUCTION

A feature common to all quantum Fermi liquids is the possibility of Cooper-pair formation, giving rise to superconductivity or superfluidity. Experimental evidence of such paired phases shows up in extended systems such as the electron gas in superconducting metals, liquid <sup>3</sup>He and possibly in neutron-star matter as well, and in finite systems such as nuclei. The theoretical frame for the description of paired systems is satisfactory, and the data confirm the model prediction that while electron Cooper pairs are formed in a singlet spin state, helium atoms choose to pair up in a triplet state. This distinction between spin channels does not apply to nuclei, since nucleons prefer a j-j coupling scheme; in neutron stars, the proton and neutron fluids coexist with different densities, which strongly determines their feasibility to constitute Cooper pairs.

To our current knowledge, a theoretical description of singlet and triplet pairing in drops of quantum liquids with single-particle states in the l-s coupling scheme has not been presented. Such an approach could be of some relevance, in view of the fact that the theoretical study of physical properties of helium drops has attracted considerable interest in spite of the scarce experimental information available. At present, variational Monte Carlo<sup>2,3</sup> and density-functional<sup>4,5</sup> calculations have been carried out to describe the ground-state properties of drops made of <sup>3</sup>He or <sup>4</sup>He atoms; some effort has also been devoted to the description of the excitation properties of these systems, especially in the case of <sup>4</sup>He.<sup>6-8</sup> For <sup>3</sup>He in the normal phase, the only available calculations of the excitation spectrum have been performed within the densityfunctional approach proposed by Stringari, using the random-phase-approximation or fluid dynamics. 11,12 The original <sup>3</sup>He density functional of Ref. 9 has been improved by a series of authors in order to accommodate in the formalism not only a quantitative description of the ground state and thermodynamical properties, such as the equation of state, but also its excitation properties, such as Landau parameters, zero sound and paramagnon propagation<sup>13,14</sup> and pairing properties,<sup>15</sup> the scope being the development of a density functional capable of describing both the ground state and the dynamics of the liquid as well as of the droplets.<sup>16</sup>

The purpose of the present work is to advance a formalism that can be of use in future applications to <sup>3</sup>He drops. For this sake, we have developed a theoretical frame to calculate the possible occurrence of triplet pairing in fermionic droplets in which a single nl shell is active. The method is applied to a constant-strength model, for which we discuss the different phase transitions that take place as the number of particles in the shell is varied. In order to fix ideas relative to the properties of superfluid droplets, we shall restrict our considerations to the case where Cooper pairs are formed within a single nl shell. This restriction is not severe on physical grounds, since mean-field calculations of <sup>3</sup>He drops<sup>4,5,16</sup> show that shell separation in the neighborhood of the Fermi level amounts to tenths of a kelvin degree, while critical temperatures in the liquid lie in the millikelvin region. Specific calculations have been carried out for a shell with orbital quantum number l = 7, which can hold at most 30 particles. In <sup>3</sup>He densityfunctional calculations<sup>5,16</sup> this occurs for example when the 1j (particle number N from 169 to 198) and 2j (N from 369 to 398) shells are being filled. Typical figures for single-particle energies of orbitals near the Fermi level are  $\epsilon_{5s} = -1818$  mK,  $\epsilon_{2j} = -1628$  mK (Fermi level), and  $\epsilon_{3h} = -1593$  mK for  $^3{\rm He}_{398}.^{16}$  These quantities would lend some support to the use of a single-shell model to describe triplet pairing in <sup>3</sup>He drops.

In Sec. II we present the general formalism here developed along the lines advanced by various authors<sup>17–19</sup> to establish the finite-system BCS model of nuclear physics, where we have incorporated the specific invariance requirements of an attractive pairing interaction acting in

the spin-triplet channel. In Sec. III we specialize the general formalism to a single-shell model and propose two choices of the gap vector which give rise to an isotropic and to an anisotropic superfluid phase. Section IV contains the formulation of the triplet-pairing problem in the single-shell model for finite temperatures. Some particular calculations are presented and discussed in Sec. V, while Sec. VI contains the summary.

## II. FORMALISM FOR PAIRING IN FINITE SYSTEMS WITHIN THE *l-s* COUPLING SCHEME

Let us consider a set of single-particle states  $|i\sigma_i\rangle$ , where

$$|i\sigma_i\rangle = |n_i l_i m_i \sigma_i\rangle, \tag{1}$$

$$|\bar{i}\sigma_i'\rangle = |n_i l_i - m_i \sigma_i'\rangle, \tag{2}$$

and an interaction that couples fermions in states  $|i\sigma_i\rangle$  and  $|\bar{i}\sigma_i'\rangle$ ,

$$H_{1} = \sum_{i,j>0,\sigma,\sigma'} \langle i\sigma_{i}\bar{i}\sigma'_{i} \mid V \mid j\sigma_{j}\bar{j}\sigma'_{j}\rangle c^{\dagger}_{i\sigma_{i}}c^{\dagger}_{\bar{i}\sigma'_{i}}c_{\bar{j}\sigma'_{j}}c_{j\sigma_{j}},$$

$$(3)$$

where  $\langle i\sigma_i \bar{i}\sigma_i' \mid V \mid j\sigma_j \bar{j}\sigma_j' \rangle$  is the antisymmetrized matrix element of the interaction. If the coupled-spin basis  $\mid SM >$  is adopted, the above interaction can be rewritten as

$$H_{1} = \sum_{i,j>0} \sum_{SM} \langle i\bar{i}SM \mid V \mid j\bar{j}SM \rangle b_{iSM}^{\dagger} b_{\bar{j}SM}, \qquad (4)$$

with the pair creation operator

$$b_{iSM}^{\dagger} = [c_{i\sigma_i}^{\dagger} c_{i\sigma_i'}^{\dagger}]_M^S \tag{5}$$

being  $b_{\overline{i}SM}$  its Hermitian conjugate. If we explicitly introduce the values of the Clebsch-Gordan coefficients involved in the coupling, we readily find (a) the antisymmetric, spin-singlet pair operator

$$b_{i00}^{\dagger} = \frac{1}{\sqrt{2}} (c_{i+}^{\dagger} c_{\bar{i}-}^{\dagger} - c_{i-}^{\dagger} c_{\bar{i}+}^{\dagger}), \tag{6}$$

and (b) the symmetric, spin-triplet operators

$$b_{i10}^{\dagger} = \frac{1}{\sqrt{2}} (c_{i+}^{\dagger} c_{i-}^{\dagger} + c_{i-}^{\dagger} c_{i+}^{\dagger}), \tag{7}$$

$$b_{i1\pm 1}^{\dagger} = c_{i\pm 1}^{\dagger} c_{i\pm 1}^{\dagger}. \tag{8}$$

In Eq. (4) we have implicitly assumed that the interaction operator V is diagonal in the coupled-spin representation. We then realize that the interaction splits into a singlet and a triplet term,

$$H_{1} = H_{s} + H_{t}$$

$$= \sum_{ij>0} \langle i\vec{i} \mid V_{0} \mid j\vec{j}\rangle b_{i00}^{\dagger} b_{\vec{j}00}$$

$$+ \sum_{ij>0} \sum_{M=0,\pm 1} \langle i\vec{i} \mid V_{1M} \mid j\vec{j}\rangle b_{i1M}^{\dagger} b_{\vec{j}1M}, \qquad (9)$$

where  $V_0$ ,  $V_{1M}$  are operators upon coordinate space once the matrix elements in spin space have been computed,

$$V_0(\mathbf{r}_1, \mathbf{r}_2) = \langle 00 \mid V(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) \mid 00 \rangle, \tag{10}$$

$$V_{1M}(\mathbf{r}_1, \mathbf{r}_2) = \langle 1M \mid V(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) \mid 1M \rangle. \tag{11}$$

The standard BCS procedure for the treatment of j-j pairing in finite nuclei,  $^{17-19}$  consists of looking for a wave function that minimizes the mean value of the total Hamiltonian  $H_0+H_1$  in the frame of the variational principle, under the constraints corresponding to conservation of the average particle number and normalization of the outcoming single-quasiparticle states. Here  $H_0$  is the original single-particle Hamiltonian whose ground state is a reference Slater determinant  $|\Phi\rangle$ ; most usually,  $|\Phi\rangle$  represents the Hartree-Fock ground state

In the present case, to generalize the standard description we might look for a variational state of the form

$$\mid \Psi \rangle = \prod_{SM} \prod_{i>0} (u_i^{SM} + v_i^{SM} b_{iSM}^{\dagger}) \mid \Phi \rangle. \tag{12}$$

Following the mathematical details of the finite-system BCS theory,  $^{17-19}$  it can be shown that the state vector  $|\Psi\rangle$  represents a vacuum for quasiparticle quasiparticle excitations,

$$|\Psi\rangle = \prod_{SM} \prod_{i>0} a_{iSM}^{\dagger} |\Phi\rangle, \tag{13}$$

where the quasiparticle operators  $a^{\dagger}, a$  are related to the original single-particle ones  $c^{\dagger}, c$  by the so-called Bogoliubov-Valatin transformation,<sup>20</sup>

$$a_{iSM}^{\dagger} = [u_i^{SM} c_{i\sigma_i}^{\dagger} - v_i^{SM} c_{\bar{i}\sigma_i'}]_M^S, \tag{14}$$

$$a_{\overline{i}SM} = [v_i^{SM*} c_{\overline{i}\sigma_i'}^{\dagger} - u_i^{SM*} c_{i\sigma_i}]_M^S. \tag{15}$$

Here the symbol  $[\ ]_M^S$  indicates that the spins of the involved operators  $c^{\dagger}$ , c add up to S, with  $\sigma_i + \sigma_i' = M$  [cf. Eq. (5)]. Furthermore, the condition that  $a^{\dagger}$ , a should be fermion operators forces the transformation matrix in Eqs. (14) and (15) to be unitary; in particular,

$$|u_i^{SM}|^2 + |v_i^{SM}|^2 = 1.$$
 (16)

We now minimize the Lagrangian function

$$L = \langle \Psi \mid H_0 + H_1 - \lambda N \mid \Psi \rangle + \sum_{i>0.SM} 2E_i[|u_i^{SM}|^2 + |v_i^{SM}|^2],$$
 (17)

where  $\lambda$  and the set of quasiparticle energies  $\{E_i\}$  are

the Lagrange multipliers for the given constraints. The variational procedure is identical to that of the finite-system BCS problem and has been reviewed in many textbooks<sup>18,19</sup> (see also Refs. 17 and 21); the total free energy  $\mathcal{F} = \langle \Psi \mid H_0 + H_1 - \lambda N \mid \Psi \rangle$  can be written as

$$\mathcal{F} = \sum_{SM} \sum_{i} 2 |v_{i}^{SM}|^{2} \tilde{\varepsilon}_{i} + \sum_{SM} \sum_{i i > 0} V_{i i j \bar{j}}^{SM} (u_{i}^{SM} v_{i}^{SM})^{*} u_{j}^{SM} v_{j}^{SM}, \qquad (18)$$

where the matrix elements in Eqs. (9)–(11) are generically denoted as  $V^{SM}_{i\bar{i}j\bar{j}}$  and

$$\tilde{\varepsilon}_i = \varepsilon_i - \lambda + V_{i\bar{i}i\bar{i}}^{SM} \mid v_i^{SM} \mid^2. \tag{19}$$

The results of the variation can be cast in terms of the relations

$$\mid v_i^{SM} \mid^2 = \frac{1}{2} \left( 1 - \frac{\tilde{\varepsilon}_i}{E_i^{SM}} \right), \tag{20}$$

$$\mid u_i^{SM} \mid^2 = \frac{1}{2} \left( 1 + \frac{\tilde{\varepsilon}_i}{E_i^{SM}} \right), \tag{21}$$

where

$$E_i^{SM} = \sqrt{\tilde{\varepsilon}_i^2 + [\Delta_i^{SM}]^2},\tag{22}$$

and the gap  $\Delta_i^{SM}$  is

$$\Delta_i^{SM} = -\sum_{i>0} V_{i\bar{i}j\bar{j}}^{SM} u_j^{SM} v_j^{SM}. \tag{23}$$

The particle number in each "spin phase" is

$$N_{SM} = 2\sum_{i} |v_{i}^{SM}|^{2}, (24)$$

and the Lagrange multiplier  $\lambda$ , representing the common chemical potential of the equilibrated phases, can be determined by the total particle-number constraint

$$N = \sum_{SM} N_{SM}.$$
 (25)

Within this philosophy, for each total-spin channel SM the variational method gives rise to the set of equations (19)–(24), which are characteristic of the finite-system BCS problem.<sup>18,19</sup>

Another approach to the problem consists of assuming that the N particles belong to the same spin channel and ask for the relative stability of the four phases; in other words, one has to search the minimum free energy of the system. It is well known<sup>21</sup> that in liquid <sup>3</sup>He, the analysis of thermodynamic stability requires the consideration of the isotropy or anisotropy of the Cooper pairs, i.e., of the way in which the total-spin axis is oriented in relative momentum space. We then note that in the spin-triplet phase the preceding formulation in terms of

three uncoupled BCS problems for  $S=1, M=\pm 1$  is not rotationally invariant, since the quasiparticle energy  $E_i$  depends upon the total-spin orientation. This is unacceptable in an unitary—i.e., rotationally invariant—state for liquid <sup>3</sup>He; similarly to the description of the infinite system, <sup>21</sup> we shall assume that in the triplet state S=1,  $E_i$  is associated to the gap matrix  $\hat{\Delta}_i$ ,

$$\hat{\Delta}_i = \begin{pmatrix} \Delta_{i++} & \Delta_{i+-} \\ \Delta_{i-+} & \Delta_{i--} \end{pmatrix}, \tag{26}$$

where we adopt the notation  $\Delta_{i\sigma_i\sigma'_i}$   $(\sigma_i + \sigma'_i = M)$  to denote the gap parameters in (23) for S = 1, by the matrix equation

$$E_i = \sqrt{\tilde{\varepsilon}_i^2 + \hat{\Delta}_i \cdot \hat{\Delta}_i^{\dagger}}.$$
 (27)

Furthermore, introducing the vector

$$\Delta_i = \left(\frac{\Delta_{i--} - \Delta_{i++}}{2}, \frac{\Delta_{i++} + \Delta_{i--}}{2i}, \Delta_{i+-}\right) \quad (28)$$

such that

$$\Delta_{i} = \begin{pmatrix} -\Delta_{ix} + i\Delta_{iy} \, \Delta_{iz} \\ \Delta_{iz} & \Delta_{ix} + i\Delta_{iy}, \end{pmatrix}, \tag{29}$$

we have

$$\hat{\boldsymbol{\Delta}}_i \cdot \hat{\boldsymbol{\Delta}}_i^{\dagger} = |\boldsymbol{\Delta}_i|^2 . \tag{30}$$

Consequently, the quasiparticle energy is a scalar

$$E_i = \sqrt{\tilde{\varepsilon}_i^2 + |\Delta_i|^2}. (31)$$

The "spin phases" appearing in the droplet are thus (a) a BCS-like phase for the spin-singlet channel, whose gap and occupation can be obtained from the system of equations (19)—(24), and (b) a spin-triplet phase characterized by a gap matrix and a scalar quasiparticle energy, with occupations (20) for pairs with total-spin projection M ( $M=0,\pm 1$ ). In the next sections we discuss some possible realizations for the gap matrix and the characterization of the corresponding "spin phase."

## III. TRIPLET PAIRING IN A SINGLE SHELL

Let us first comment on pair formation and pair counting in a single l shell. For the 2l + 1 magnetic substates with two spin occupation possibilities each, we recog-(i) If  $M = \pm 1$ , the pair denize the following facts: generacy is  $\Omega_{\pm 1} = l$ , since the sublevel with m = 0does not participate in the formation of Cooper pairs  $(m, \sigma = \pm), (-m, \sigma = \pm);$  (ii) if M = 0, the projection m = 0 yields one pair with opposite spin projections and thus  $\Omega_0 = 2l + 1$ . Note in passing that the spin pairs  $(\sigma \sigma') = (+-)$  and (-+), both in magnetic levels (m, -m), appear in the symmetric or antisymmetric combinations for S = 1, 0. It is then clear that the maximum number of particles that can couple to either S=1 with the three total projections or to S=0 is  $N_{\text{max}} = 2(2l+1)$ , i.e., the full degeneracy of the shell.

It is convenient as well to establish how the total energy for the N-fermion system is computed. Because of the arbitrariness in the assignment of a value to the single-particle energy  $\varepsilon$  of the shell in the single-shell model, we rather calculate the free-energy excess  $\mathcal{E} = \mathcal{F} - N\varepsilon$ . On the one hand, if one can neglects<sup>18</sup> the "self-energy" contribution proportional to the occupation rate in (19), the single-particle energy excess is simply

$$\mathcal{E}_0 = -N\lambda,\tag{32}$$

while from Eqs. (18), (20), (21), and (23) we can write the pairing energy as

$$\mathcal{E}_P = -\sum_{m>0} \frac{\hat{\Delta}_m \cdot \hat{\Delta}_m^{\dagger}}{2E_m}.$$
 (33)

The free-energy excess is thus  $\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_p$ .

Within this framework, we first normalize the gap vector according to

$$\Delta_{nlm} = \Delta \mathbf{f}(m), \tag{34}$$

where  $\Delta$  is an average over the shell,

$$|\Delta|^2 = \frac{1}{2l+1} \sum_{m=-l}^{l} |\Delta_{nlm}|^2,$$
 (35)

i.e.,

$$\frac{1}{2l+1} \sum_{m=-l}^{l} |\mathbf{f}(m)|^2 = 1.$$
 (36)

One may say that Eq. (36) is the translation to finite systems of the normalization relationship  $\int (d\Omega/4\pi) |\mathbf{f}(\Omega)|^2 = 1$  adopted in the case of liquid <sup>3</sup>He.<sup>21</sup>

We can see that the parameter  $\Delta$  satisfies a BCS-like equation; <sup>17-19</sup> indeed, if the matrix elements  $V_{i\bar{i}j\bar{j}}$  do not depend upon the spin projection M, the components of the gap vector  $\Delta$  verify Eq. (23), namely,

$$\Delta_{nlm} = \Delta \mathbf{f}(m)$$

$$= -\sum_{m'>0} V_{m-mm'-m'} \frac{\Delta}{2E_{m'}} \mathbf{f}(m'). \tag{37}$$

If we now perform a scalar product with f(m) and average over the shell, we obtain

$$1 = -\frac{1}{2l+1} \sum_{m} \sum_{m'>0} V_{m-mm'-m'} \frac{\mathbf{f}(m) \cdot \mathbf{f}(m')}{2E_{m'}}$$
$$= -\sum_{m>0} \frac{\tilde{V}_m}{2E_m}, \tag{38}$$

where

$$E_m^2 = \tilde{\varepsilon}^2 + \Delta^2 \mid \mathbf{f}(m) \mid^2 \tag{39}$$

and the effective matrix element appearing in Eq. (38) is

$$\tilde{V}_m = \frac{\mathbf{f}(m)}{2l+1} \sum_{m'} V_{m'-m'm-m} \mathbf{f}(m'). \tag{40}$$

Equation (38) together with the particle-number conservation rule  $N=2\sum_{m=-l}^{l}v_m^2$  given by (24) completely states the triplet-pairing problem in terms of the unknowns  $\Delta$  and  $\lambda$ . It should be kept in mind that in the spin-triplet phase, the interaction matrix elements must be spatially antisymmetric. On the other hand, it is also worthwhile noting that the effective matrix element of the present formulation generalizes to finite systems, the angular averages entering the gap equation for the translationally invariant liquid. <sup>21</sup>

Different phases for triplet pairing in droplets correspond to different choices for the gap vector  $\mathbf{f}(m)$ . Similarly to the case of the infinite system, we may intuitively expect that this vector defines the direction along which the pair of particles in states  $|i\sigma_i\rangle$  and  $|\bar{i}\sigma_i'\rangle$  possesses total-spin projection M=0. In liquid <sup>3</sup>He, the gap vector is usually denoted as d(n) and is expressed in terms of the normalized relative momentum vector  $\mathbf{n} = \mathbf{k}/k$  by the relation  $d_i = \sum_{\alpha} d_{\alpha i} n_{\alpha}$ . The determination of the free-energy minima and the identification of the unitary phases requires an analysis of the quadratic and quartic invariants entering the fourth-order expansion of the Tdependent free energy in terms of the gap, in the vicinity of the transition temperature; it turns out that the different unitary phases correspond to the matrix  $d_{\alpha i}$  being a one-, two-, or three-dimensional unit matrix.<sup>22,23</sup> In the present case, since the dynamical group of the droplet is a nonconmutative one, opposite to the translational group for the liquid, there is no obvious formulation for the gap vector in terms of generators of the rotation algebra; furthermore, the axial component of the angular momentum of each particle is the only observable compatible with the shell specification. With this in mind and in the spirit of attempting a comparison among several alternatives, in what follows we will build up possible descriptions for spin-triplet superfluid phases in drop focusing upon tentative isotropic and anisotropic gaps, postponing a formal investigation of the existence of minima of the free energy and their geometrical characterization.

## A. Isotropic phase

The superfluid Balian-Werthamer (BW) (Ref. 24) phase in liquid  ${}^{3}$ He corresponds to the three-dimensional  $d_{\alpha i}$  matrix, with gap vector  $\mathbf{f}^{\mathrm{BW}}(\mathbf{n}) = \mathbf{n}$ . We then force an isotropic unitary phase in a finite system, taking

$$\mathbf{f}_I(m) = \frac{1}{\sqrt{3}}(1, 1, 1). \tag{41}$$

The effective matrix element in Eq. (40) is then

$$\tilde{V}_{m}^{I} = \frac{1}{(2l+1)} \sum_{m'} V_{m'-m'm-m}, \tag{42}$$

and the quasiparticle energy, which is independent of m, can be computed from (38) as

$$E_m^I \equiv E_I = -\frac{1}{2} \sum_{m'>0} \tilde{V}_{m'}^I. \tag{43}$$

In addition, from the particle-number condition (24) one gets

$$v_m^2 \equiv v^2 = \frac{N}{2\Omega},\tag{44}$$

with  $\Omega$  the pair degeneracy 2l+1. Using Eq. (20), we easily obtain

$$\tilde{\varepsilon}_I = E_I \left( 1 - \frac{N}{\Omega} \right) \tag{45}$$

and

$$\Delta_{I} = \frac{1}{2\Omega} \left| \sum_{m>0} \tilde{V}_{m}^{I} \right| \sqrt{N(2\Omega - N)}$$

$$\equiv \frac{|G_{I}|}{2} \sqrt{N(2\Omega - N)}.$$
(46)

The above Eqs. (44)—(46) are identical to the well-known ones derived in the finite-system BCS formalism for the case of pairs in a single j shell<sup>18,19,25</sup> with a constant pairing strength G. In the present case, the equivalent constant is

$$G_I = \frac{1}{\Omega} \sum_{m>0} \tilde{V}_m^I. \tag{47}$$

In view of the discussion in this section, the pairing energy becomes

$$\mathcal{E}_p^I = \frac{|\Delta_I|^2}{G_I}.\tag{48}$$

## B. Anisotropic phase

From the theoretical viewpoint,  $^{22,23}$  in liquid  $^3$ He there may exist three independent anisotropic phases characterized by the gap vectors (a) for the one-dimensional (polar) case,  $\mathbf{f}_{1D}(\mathbf{n}) = \sqrt{3}(0,0,n_z)$ ; (b) for the two-dimensional (planar) case,  $\mathbf{f}_{2D}(\mathbf{n}) = \sqrt{\frac{3}{2}}(n_x,n_y,0)$ ; and (c) for the Anderson-Brinkman-Morel (ABM or axial) phase,  $\mathbf{f}_{ABM}(\mathbf{n}) = \sqrt{\frac{3}{2}}(n_x + in_y,0,0)$ .

To compare with the preceding isotropic case, let us then choose an anisotropic gap vector for the droplet,

$$\mathbf{f}_{A}(m) = \sqrt{\frac{3}{l(l+1)}}(0,0,m). \tag{49}$$

This choice is arbitrary except for the fact that it resembles the one-dimensional liquid phase, which is the only one from the above list that can be mapped onto the available observables of a finite system, namely, the angular momentum projection of each paired particle in the shell. One can realize as well that the superfluid phase thus constructed is sixfold degenerate with respect to the possibilities of filling up the components of  $\mathbf{f}_A(m)$  with quantities proportional to m, keeping the overall nor-

malization. It is easy to verify that the effective matrix element is

$$\tilde{V}_{m}^{A} = \frac{3m}{(2l+1)l(l+1)} \sum_{m'} m' V_{m'-m'm-m},$$
 (50)

and that the quasiparticle energy is now m dependent,

$$E_m^A = \sqrt{\tilde{\varepsilon}_A^2 + \frac{3m^2}{l(l+1)}\Delta_A^2},\tag{51}$$

which leads us into a numerical scheme, namely,

$$1 + \sum_{m>0} \frac{\tilde{V}_m^A}{2E_m^A} = 0, (52)$$

$$N - \Omega + \tilde{\varepsilon}_A \sum_{m} \frac{1}{E_m^A} = 0. \tag{53}$$

The pairing energy reads [cf. Eq. (33)]

$$\mathcal{E}_p^A = -3 \frac{\Delta_A^2}{2l(l+1)} \sum_{m>0} \frac{m^2}{E_m^A}.$$
 (54)

# IV. SPIN TRIPLET PHASE FOR FINITE TEMPERATURES

The formulation of the finite-temperature pairing theory for Fermi liquids has been already presented in the literature, <sup>21</sup> as well as the corresponding extension of the BCS theory to nuclei. <sup>26</sup> The derivation procedure is identical to the zero-temperature case, with the thermodynamic free energy (in the grand canonical ensemble, i.e., the grand potential) as the functional to be minimized. For the spin-triplet phase, the grand potential reads

$$\mathcal{F} = \mathcal{E}_0 + \sum_{m,m'>0} V_{m-mm'-m'}^{SM} \left( u_m v_m \tanh \frac{\beta E_m}{2} \right) \times \left( u_{m'} v_{m'} \tanh \frac{\beta E_{m'}}{2} \right) - T \sum_m \ln(1 + e^{-\beta E_m}), \tag{55}$$

where  $\beta = 1/T$  is the inverse temperature and the last term is the total entropy. Here the gap is

$$\Delta_m^{SM} = -\sum_{m'>0} V_{m-mm'-m'}^{SM} u_{m'} v_{m'} \tanh \frac{\beta E_{m'}}{2},$$
 (56)

while u, v, and the chemical potential  $\lambda$  are determined by the same equations as for the zero-temperature case [cf. Eqs. (19)–(24)]. Accordingly, for the single l shell, the gap equation acquires the form

$$1 = -\sum_{m>0} \frac{\tilde{V}_m}{2E_m} \tanh \frac{\beta E_m}{2}.$$
 (57)

We now discuss the specific details of the triplet isotropic (I) and anisotropic (A) phases of Sec. III.

#### A. Isotropic phase

From Eq. (57) and the conditions described in Sec. III A we obtain a trascendental equation for the quasiparticle energy,

$$\tanh\frac{\beta E_I}{2} = -\frac{2E_I}{\Omega G_I},\tag{58}$$

where  $G_I$  is the effective coupling constant defined in Eq. (47). Now, the graphical analysis of Eq. (58) clearly shows the existence of an N-independent critical temperature

$$T_{\rm crit}^I = \frac{\Omega \mid G_I \mid}{4},\tag{59}$$

below which there exists a nonvanishing quasiparticle energy  $E_I$  that can be numerically found. According to Eq. (56), the gap is

$$\Delta_I(T) = \Delta_I(0) \tanh \frac{\beta E_I}{2},\tag{60}$$

where  $\Delta_I(0)$  is the zero-temperature gap given in (46). The pairing energy then reads

$$\mathcal{E}_p^I = \frac{\Delta_I^2(T)}{G_I}.\tag{61}$$

## B. Anisotropic phase

The numerical calculation to be performed is the solution of Eqs. (53) and (57). In view of Eqs. (33) and (56), we recognize that the pairing contribution to the grand potential can be written as

$$\mathcal{E}_{p}^{A} = -\frac{3}{2} \frac{\Delta_{A}^{2}}{l(l+1)} \sum_{m>0} \frac{m^{2}}{E_{m}^{A}} \tanh \frac{\beta E_{m}^{A}}{2}$$
 (62)

[cf. Eq. (54)], while the single-particle free-energy excess  $\mathcal{E}_0$  is given by (32) and the entropy has to be computed as indicated in (55).

### V. CONSTANT PAIRING STRENGTH MODEL

In this section we present a specific model for the interaction, inspired in the popular "constant BCS pairing" of nuclear physics.  $^{18,19,25}$  In this model, one assumes that the matrix elements in the single shell are identical to a negative constant G; in the present case, keeping in mind that the spatial matrix elements must be antisymmetric, the extension of the above model can be explicitly given by the choice

$$V_{m-mm'-m'} = V_{-mm-m'm'}$$

$$= G = -V_{-mmm'-m'} = -V_{m-m-m'm'},$$
(63)

with the corresponding assignments for the Hermitianconjugated matrix elements. We now carry on the detailed analysis of each spin-triplet phase.

#### A. Isotropic phase

According to Eq. (47), the effective strength can be computed as follows:

$$G_I = \frac{2}{\Omega^2} \sum_{m,m'>0} G,\tag{64}$$

which yields

$$G_I = 2G \left(\frac{l}{\Omega}\right)^2. \tag{65}$$

The values of the quasiparticle energy  $E_I$ , fractional occupation  $v^2$ , gap  $\Delta_I$ , and pairing free energy  $\mathcal{E}_p^I$  are then given by Eqs. (43), (44), (46), and (48), respectively, which are just the "constant BCS pairing" results.

## B. Anisotropic phase

In this case the effective matrix element  $\tilde{V}_m^A$  is

$$\tilde{V}_{m}^{A} = \frac{2}{\Omega} \sum_{m'>0} \frac{3mm'}{l(l+1)} G, \tag{66}$$

which gives

$$\tilde{V}_m^A = \frac{3Gm}{\Omega}.\tag{67}$$

The calculation then proceeds numerically by solving Eqs. (52) and (53). It is also clear that, as in the former case, all energies are proportional to the pairing strength.

As an illustration of the predictions of this formalism, we present in Figs. 1-5 calculations performed under

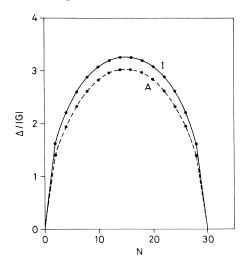


FIG. 1. Zero-temperature gap as a function of the particle number in the shell. Solid line: isotropic phase. Dashed line: anisotropic phase.

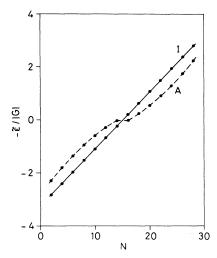


FIG. 2. Zero-temperature chemical potential referred to the unperturbed single-particle level energy, as a function of the particle number in the shell. Solid line: isotropic phase. Dashed line: anisotropic phase.

the above prescriptions in an l=7 shell, where the maximum number of particles to be paired is 30. Figures 1–3, respectively, display the zero-temperature results for the gap  $\Delta$ , the chemical potential  $\lambda=-\tilde{\varepsilon}$  (thus referred to the unperturbed single-particle level energy  $\varepsilon$ ), and the free-energy excess  $\mathcal{E}$ , in units of the coupling constant  $\mid G\mid$ ; in these figures, the lines connecting the points are to guide the eye. Figures 4 and 5, respectively, exhibit the T-dependent gap and the free-energy excess in units of  $\mid G\mid$  for N=6, N=10, and N=20 particles; it should be noted that the gap is the same for both N=10 and N=20, due to symmetry about midshell.

From inspection of the figures, we can appreciate the

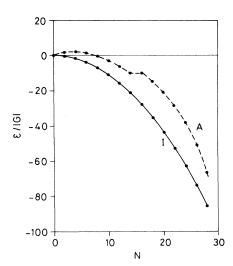


FIG. 3. Zero-temperature free-energy excess as a function of the particle number in the shell. Solid line: isotropic phase. Dashed line: anisotropic phase.

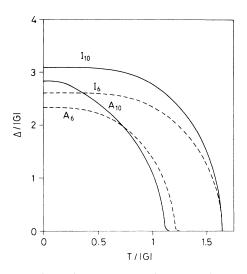


FIG. 4. T-dependent gap as a function of temperature for N=6 (dashed lines) and N=10 (solid lines) particles in the shell. I stands for the isotropic phase and A for the anisotropic one.

following features. First, in the zero-temperature situation the overall shape of each set of curves is rather similar for both triplet phases; the largest deviations occur near midshell. The isotropic phase is more strongly bound than the anisotropic one, for all particle numbers. The energy of the anisotropic phase displays an inflection point at midshell; such an appearance can be traced to the behavior of the chemical potential, since we realize from Fig. 2 that, while in the isotropic phase this parameter is a linear function of the particle number [cf. Eq. (45)], in the anisotropic phase it resembles, as a function of N, an odd parabola centered at midshell. It is noticeable that for small particle numbers, i.e., N < 8, the anisotropic free-energy excess is positive; the reason

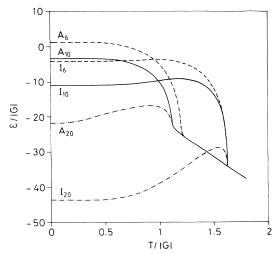


FIG. 5. Free-energy excess as a function of temperature for N=6 (dashed lines), N=10 (solid lines), and N=20 (dot-dashed lines) particles in the shell. I stands for the isotropic phase and A for the anisotropic one.

is that in spite of the fact that the pairing energy  $\mathcal{E}_p^A$  is negative, its magnitude is not sufficient to compensate the positive single-particle energy excess  $\mathcal{E}_0=N\mid\lambda\mid$ ; thus, on thermodynamical grounds a droplet with those particle numbers subjected to a constant attractive pairing interaction is not bound. However, it should be kept in mind that this effect is an artifact of considering the single shell as constituting the whole system; in fact, actual computations for drops with either the 1j or 2j shell active show that these drops are indeed bound when one takes explicitly into account the remaining shells which do not contribute to the formation of pairs.

Second, regarding the temperature-dependent gap and chemical potential (this latter not shown), one encounters the typical behavior of the order parameter in a secondorder phase transition; apparently, in the anisotropic case there is not a sharp cutoff but a smooth approach to zero, however in a much smaller scale of gap values than the characteristic scale of the current plot. A critical temperature for the anisotropic phase can be estimated, for example, searching where the gap drops below 0.01 times the zero-temperature value (see Fig. 4). From the calculations it can be verified that  $T_{\rm crit}^A$  depends upon the particle number in the shell and is always smaller than  $T_{\rm crit}^{I}$ , where the latter is given by (59); furthermore, the anisotropic critical temperature decreases as one evolves from an empty to a half-filled shell and behaves symmetrically with respect to midshell. The analysis of the results for the whole set of particle numbers shows that  $T_{\text{crit}}^{A}$  varies between 1.4 and 1.1 times | G | for N varying between 2 and 14.

Concerning the behavior of the free-energy excess, we first note that for  $T>T_{\rm crit}^{I,A}$  the corresponding free energy is a linearly decreasing function of temperature; this is precisely the contribution of the entropy term TS, with an entropy  $S = 2\Omega$  ln 2. In addition, we see in Fig. 5 that for N = 6 and N = 10 three different regimes appear: (i) the normal phase for  $T > T_c^I$ ; (ii) as the isotropic phase becomes a possibility for temperatures smaller than  $T_c^I$ , the normal phase is still thermodynamically more convenient; (iii) when the transition from a normal to a superfluid phase takes place, the anisotropic phase is the most stable. The situation is reversed for temperatures below the crossing at  $T_{\rm cross} \simeq \mid G \mid$ , where isotropy becomes preferential. We then realize that there exists a temperature interval where a stable drop can be found in an anisotropic paired phase, namely,  $T_{\text{cross}} \leq T \leq T_{\text{crit}}^A$ . However, for N=20 only two regimes are apparent, since the anisotropic phase is never a thermodynamical choice for the system. Indeed, while for each phase the gap is the same function of T for N=10and N = 20, the differences in the free-energy excess for these particle numbers are entirely due to the unperturbed energy  $\mathcal{E}_0$  since the chemical potential reverses its sign at midshell. The numerical data show that this is a feature of each pair of particle numbers  $(N, 2\Omega - N)$ ; in other words, as the number of particles is higher than the pair degeneracy, the anisotropic phase cannot be reached at any temperature.

### VI. CONCLUSIONS

Inspired in the finite-system BCS theory of nuclear physics, in this work we have constructed a formalism to describe triplet pairing in fermionic droplets, both at zero and at finite temperature. Although the experimental confirmation of triplet pairing in liquid <sup>3</sup>He raises <sup>3</sup>He drops as the major candidates to exhibit such a superfluid behavior, other natural systems such as atomic nuclei may be subjected as well to this type of calculations. The main difficulty encountered in closing the general theoretical frame lies in the characterization of the geometry of the gap matrix; at this point, since a rigorous answer to questions regarding the location of the free-energy minimum demands a deeper analysis of the transition region,<sup>21</sup> we have restricted ourselves to indicate two simple appearances for an isotropic and an anisotropic gap matrix in a single-shell model. To fix ideas to a stronger degree, we have chosen a constant attractive pairing interaction and carried out some particular examples.

As a general characteristic of all calculations performed within the present model, one finds that the isotropic triplet phase is, at low temperatures, thermodynamically more stable than the anisotropic one. In this context, as we attempt a comparison between the singlet (BCS) and the triplet phases, we find that the effective pairing strength in the latter is reduced, with respect to the BCS strength. On the other hand, since  $|G_I| < |G| \equiv |G_{\text{BCS}}|$ and every energy in the formalism is proportional to the coupling constant, the factor  $2(l/\Omega)^2$  in (65) gives the relative scale between the BCS and the I phases in the droplet. For given G, the BCS phase will be the most stable. Of course, this is a feature of the single-shell model with a constant pairing interaction and is not necessarily expected to remain in actual droplets where the pairing matrix elements have to be explicitly computed out of some particle-particle interaction. However, even within the severe limitations of the current approach, it is noticeable that the possibility of reaching an anisotropic state at some finite temperature is restricted to particle numbers below midshell. In some way, this feature may remind one the characteristic of the second-order phase transition in liquid <sup>3</sup>He; namely, the fact that the phase to be reached as the temperature is lowered is the anisotropic ABM one for pressures above the policritical point (for zero magnetic field), while the isotropic BW state shows up in the low-pressure region.

## ACKNOWLEDGMENTS

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(1992).

- <sup>1</sup>G. Scoles, in *The Chemical Physics Properties of Atomic* and *Molecular Clusters*, Proceedings of the International School of Physics "Enrico Fermi," Course CVII, Varenna, Italy, 1988 (North-Holland, Amsterdam, 1991).
- <sup>2</sup>V. R. Pandharipande, S. C. Pieper, and R. B. Wiringa, Phys. Rev. B **34**, 4571 (1986).
- <sup>3</sup>D. S. Lewart, V. R. Pandharipande, and S. C. Pieper, Phys. Rev. B **37**, 4950 (1988).
- <sup>4</sup>S. Stringari and J. Treiner, J. Chem. Phys. 87, 5021 (1987).
  <sup>5</sup>S. Weisgerber and P.-G. Reinhard, Z. Phys. D 23, 275
- <sup>6</sup>S. A. Chin and E. Krotscheck, Phys. Rev. Lett. **65**, 2658 (1990).
- <sup>7</sup>M. V. Rama and K. B. Whaley, Phys. Rev. Lett. **64**, 1126 (1990).
- <sup>8</sup>M. Casas and S. Stringari, J. Low Temp. Phys. **79**, 135 (1990).
- <sup>9</sup>S. Stringari, Phys. Lett. **107A**, 36 (1985).
- <sup>10</sup>Ll. Serra, J. Navarro, M. Barranco, and N. van Giai, Phys. Rev. Lett. **67**, 2311 (1991).
- <sup>11</sup>M. Barranco, E. S. Hernández, and C. E. Vignolo, Z. Phys. D **25**, 233 (1993).
- <sup>12</sup>S. Weisgerber, Ph.D. thesis, University of Erlangen, Germany, 1992.
- <sup>13</sup>C. García-Recio, J. Navarro, N. van Giai, and L. L. Salcedo,

- Ann. Phys. (N.Y.) 214, 293 (1992).
- <sup>14</sup>S. Weisgerber and P.-G. Reinhard, Phys. Lett. A **158**, 407 (1991).
- <sup>15</sup>E. S. Hernández, M. Barranco, and A. Polls, Phys. Lett. A 117, 119 (1992).
- <sup>16</sup>M. Barranco, E. S. Hernández, D.M. Jezek, J. Navarro, and Ll. Serra (unpublished)
- <sup>17</sup>S. T. Belyaev, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. **31**, No. 11 (1959).
- <sup>18</sup>D. S. Koltun and J. M. Eisenberg, Quantum Mechanics of Many Degrees of Freedom (Wiley-Interscience, New York, 1988).
- <sup>19</sup>P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer-Verlag, Berlin, 1980).
- <sup>20</sup>N. N. Bogoliubov, Nuovo Cimento **7**, 794 (1958).
- <sup>21</sup>A. J. Leggett, Rev. Mod. Phys. **47**, 331 (1975).
- <sup>22</sup>N. D. Mermin and G. Stare, Phys. Rev. Lett. **30**, 1135 (1973).
- <sup>23</sup>W. F. Brinkman and P. W. Anderson, Phys. Rev. A 8, 2732 (1973).
- <sup>24</sup>R. Balian and N. R. Werthamer, Phys. Rev. **131**, 1553 (1963).
- <sup>25</sup>A. M. Lane, *Nuclear Theory* (Benjamin, New York, 1964).
- <sup>26</sup>M. Sano and S. Yamasaki, Prog. Theor. Phys. **29**, 397 (1963).