Cooper pairing with finite angular momentum via a central attraction: From the BCS to the Bose limits

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In the context of a simple model featuring an explicit, *central* interaction potential, and using a standard functional-integral technique, we study superconductivity with angular momentum quantum number $l=2$ as an emergent property of the many-body system. Our interaction potential is attractive at a finite distance r_0 , and the breaking of the rotational symmetry is the result of an interplay between $r₀$ and the interparticle distance *rs* . This interplay is generic to interactions of this type and is responsible for the existence of *d*-wave pairing for a range of densities. However, we find that $l=2$ pairing takes place only in the BCS limit. In contrast, as the Bose-Einstein (BE) limit is approached the internal energy of the "preformed pairs" becomes the dominant contribution and there is a quantum phase transition in which the *s*-wave symmetry is restored. We also find that the limiting value of the critical temperature is $k_B T_c \rightarrow 3.315 \hbar^2/2m^*$ $\left[\frac{n}{2}(2l+1)\right]^{2/3}$, which coincides with the usual result only for $l=0$; for $l>0$, it differs in the degeneracy factor $1/(2l+1)$, which lowers T_c . Our results thus place constraints on exotic pairing in the BE limit, while at the same time indicating a particularly interesting route to pairing with $l > 0$ in a BCS superconductor.

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I. INTRODUCTION

It is a surprising consequence of BCS theory¹ that certain *central* interaction potentials $V(|\mathbf{r}-\mathbf{r}'|)$ lead to Cooper pairing with a finite value of the angular momentum, thus breaking the rotational symmetry of the continuum.² The phenomenon is analogous to what happens in ''Hubbard'' models with attraction between nearest neighbors for which, as is well known,³ *d*-wave pairing can break the symmetry of the crystal lattice. However, it is especially interesting in the original context² of a continuum model, because of the contrast with the well-known theorem⁴ for two-body pairing in real space, which demands that the ground state minimize the orbital angular momentum. This rotational symmetry breaking is thus a many-body effect, and one expects that in the limit of low densities and strong attraction, when the BCS ground state is a Bose-Einstein (BE) condensate of nonoverlapping pairs,^{5–8} the rotational symmetry of the system is restored. However, until now investigations of the BCS to Bose crossover for non-*s*-wave pairing were performed either in the context of lattice models (see Ref. 3 for a review and Refs. $9-14$ for some examples of recent work) or for the anisotropic interaction potential of Ref. 15.16

In this paper we take a slightly different approach by studying a continuum model, but choosing to work with an explicit, *central* interaction potential $V(|\mathbf{r}-\mathbf{r}'|)$ which can lead to pairing with more than one value of the angular momentum: the " δ -shell" potential.^{17,18} The resulting " δ -shell" model (DSM) captures, in an idealized way, the essential feature leading to Cooper pairing with a finite value of the angular momentum, namely, being attractive at a welldefined, finite distance. 19 Thus we expect some of the novel features that we shall describe, pertaining to the mechanisms by which the rotational symmetry is broken in the BCS limit and restored in the BE limit, to be generic to a large class of central effective interactions. In particular we shall see that for such models the evolution of a BCS superconductor with exotic pairing towards the BE limit involves a phase transition in which the symmetry of the superconducting order parameter is increased. This adds to the work by Babaev and Kleinert²⁰ who also found, in the context of a chiral Gross-Neveu model, a phase transition associated with the BCS to Bose crossover. However, the nature of the phase transition that we describe here is quite different, as it takes place in the superconducting state, while that of Babev and Kleinert corresponds to the formation of preformed pairs in the normal state.

II. δ-SHELL MODEL

The first discussions of exotic Cooper pairing² took place in the context of the weak-coupling theory of superfluid ³He. It was assumed that there existed a central, nonretarded interaction potential $V(|\mathbf{r}-\mathbf{r}'|)$ acting between particles at positions \bf{r} and \bf{r}' . One then writes

$$
V(\mathbf{k} - \mathbf{k}') = \sum_{l' = 0}^{\infty} K_{l'}(|\mathbf{k}|, |\mathbf{k}'|)(2l' + 1)P_{l'}(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'), \quad (1)
$$

where $V(\mathbf{k}-\mathbf{k}') \equiv \int d^3 \mathbf{r} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}} V(\mathbf{r})$, and finds that each of the terms in this series leads to pairing with a different value of the angular momentum quantum number *l*. As it can, and has been, argued, in the weak-coupling limit one can approximate

$$
V(\mathbf{k} - \mathbf{k}') \approx K_l (2l + 1) P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'), \tag{2}
$$

where l is the value of l' for which the coupling constant on the Fermi surface,

$$
K_{l'} \equiv K_{l'}(k_F, k_F), \tag{3}
$$

is largest. The approximate form (2) of the potential $V(\mathbf{k})$ $-{\bf k}'$) is, for $l>0$, anisotropic, and it leads to pairing with finite angular momentum quantum number l (see Ref. 2). For $l=0$, it reduces to the BCS "contact potential,"¹ leading to *s*-wave pairing. Although introduced in the context of a weak-coupling theory, the contact potential has often been used to study the BCS to Bose crossover.²¹⁻³⁰ Similarly, Stintzing and Zwerger have considered a simplified potential of the form (2) with $l=2$ to study the BCS to Bose crossover for pairs with $d_{x^2-y^2}$ symmetry¹⁵ (but in two dimensions and with the additional assumption of separability to make it more tractable). One of the key results of this later work¹⁵ was that the critical temperature is given, in the BE limit, by the same expression as in the s -wave case^{8,22,23}:

$$
k_B T_c \approx 3.315 \frac{\hbar^2}{2m^*} \left(\frac{n}{2}\right)^{2/3} \text{ for } s \text{ and } d_{x^2-y^2} \text{ pairing.}
$$
\n(4)

Although very useful, the above approach is not appropriate to study the question that we are interested in here, since it introduces a particular pairing symmetry at the level of the interaction potential. In contrast, we want to find pairing with $l > 0$ as an emergent property of the many-body system. Moreover, we would expect, on the basis of the above arguments, to recover $l=0$ pairing in the BE limit, in which the internal structures of the Cooper pairs are independent. This physics seems also to be absent from those studies, as Eq. (4) suggests that the critical temperature is degenerate for *s* and $d_{x^2-y^2}$ superconductivity.

An alternative strategy is to do the calculations taking the full r dependence of $V(r)$ into account. A study of this type was carried out by Andrenacci *et al.*¹¹ who took a Gaussian form for $V(r)$. This allowed them to investigate the properties of the crossover at finite densities (in contrast, as is well known, the procedure required to regulate the ultraviolet divergences associated with simplified potentials of the form (2) at all couplings is only valid in the dilute limit³¹). They also considered the highly idealized separable potential introduced in the seminal paper by Nozières and Schmitt Rink,⁸ which has been employed in several other instances^{29,30} on account of its mathematical simplicity (but note that this is not, strictly speaking, a central potential). However, in either case there was no rotational symmetry breaking: even at high densities they only obtained *s*-wave superconductivity (the discussion of $d_{x^2-y^2}$ superconductivity in Ref. 11 is based on a lattice model).

On the other hand, a simple argument 19 based on the BCS "gap equation" suggests that *l*. > 0 Cooper pairing is associated with central potentials *V*(*r*) that are nonmonotonic functions of *r*, with maximum attraction near some finite distance $r \sim r_0$ >0. The δ -shell potential was proposed in Ref. 19 as the simplest form of $V(r)$ that has this feature:

$$
V(|\mathbf{r} - \mathbf{r}'|) = -g \delta(|\mathbf{r} - \mathbf{r}'| - r_0). \tag{5}
$$

The resulting DSM can be regarded as the continuum analog of the lattice model with nearest-neighbor attraction dis-

FIG. 1. The δ -shell interaction potential. *Left*: the two particles attract each other only when each of them lay on a thin shell, of radius r_0 , centered on the other one. *Right*: the δ -shell interaction potential can be regarded as an approximation to any central potential that is attractive only near some distance r_0 (see text).

cussed in Refs. 3,10–12, and 14, for example. But note that in the DSM the distance r_0 at which the fermions attract each other is a free parameter that can be varied continuously, and the noninteracting dispersion relation is that of free fermions with an effective mass *m**.

The δ -shell potential can also be considered an approximation to any central potential that is attractive only within a range of distances centred at r_0 , of width $r_c \ll r_0$, since Eq. (5) is equivalent to performing, in the general expression

$$
K_{l}(|\mathbf{k}|,|\mathbf{k}'|) = (-1)^{l} \int_{0}^{\infty} dr 4 \pi r^{2} j_{l}(|\mathbf{k}|r) V(r) j_{l}(|\mathbf{k}'|r),
$$
\n(6)

valid for any central potential $[j_l(x)]$ denotes a spherical Bessel function, the approximation

$$
\int_0^\infty dr \ 4\pi r^2 \ j_l(|\mathbf{k}|r) V(r) j_l(|\mathbf{k}'|r)
$$

$$
\approx r_c \ 4\pi r_0^2 \ j_l(|\mathbf{k}|r_0) V(r_0) j_l(|\mathbf{k}'|r_0), \tag{7}
$$

which corresponds to taking the limit $r_c \rightarrow 0$ while keeping $V(r_0) \times r_c = \text{const} \equiv -g$ (*g* thus has dimensions of energy \times length). A particularly simple example of this is the square well of Fig. 1.

The two-body problem associated with the δ -shell potential is very well known (see Refs. 17 and 18, for example). In particular, it can bind a pair in free space with any value of $l=0,1,2,...$. To simplify matters, we will assume that the attraction takes place between particles with opposite spins. Finally, in **k** space the δ -shell potential is given by $V(\mathbf{k})$ $(-\mathbf{k}') = -g4\pi r_0^2 \sin(|\mathbf{k}-\mathbf{k}'|r_0)/|\mathbf{k}-\mathbf{k}'|r_0$, from which it is evident that it reduces to the contact potential in the limit $r_0 \rightarrow 0$ (keeping $g 4 \pi r_0^2$ equal to $-K_0$). Interestingly, the δ -shell potential, for any finite r_0 , does not display the ultraviolet divergences affecting the contact potential.

We will study the BCS to Bose crossover in this new model using the standard functional-integral technique of Refs. 22,23,31, and 32. At zero temperature, it implies a description of the system in the saddle-point approximation, which amounts to using the BCS ground state³¹ (as in Refs. $7,8,10,11$, and 14, for example). Thus our results for the ground state will be approximate, but of variational significance. At the critical temperature, Gaussian fluctuations about the saddle point are taken into account as in Refs. 15,22, and 23 [as is well known³¹ this is equivalent to the random-phase-approximation-like (RPA-like) diagrammatic technique introduced by Nozieres and Schmitt-Rink δ (NSR). This approach is rather limited in that, in the strong-coupling limit, it neglects interactions between the preformed pairs, existing above T_c , and so it can only describe the effect of fluctuations on the superconducting instability at low densities.26,27 Nevertheless, as we shall see it is enough to discuss the rotational symmetry breaking in the weakcoupling limit, in which the fluctuations are negligible, as well as the mechanism by which the critical temperature becomes larger for *s*-wave pairs in the BE limit (at strong coupling *and* low densities). The application of these standard methods to the DSM is fairly straightforward, so we will quote here only the key expressions; further details can be found in Ref. 33.

Our model has four parameters: the distance r_0 at which the attraction takes place, the coupling constant *g*, the density of fermions *n*, and their mass *m**. In principle, the BCS ground state can be characterized by the dependence of the zero-temperature gap function Δ_k and chemical potential μ on these four parameters. Likewise, the superconducting instability can be described by giving the critical values of the temperature T_c and chemical potential μ_c in terms of r_0, g, n, m^* . However, the DSM has the remarkable property that the four energies $\Delta_{\mathbf{k}}$, μ , $k_B T_c$, μ_c , rescaled by the "localization energy" $\varepsilon_0 = \hbar^2 / 2m^* r_0^2$ (which we will denote $\tilde{\Delta}_{\tilde{k}}$, $\tilde{\mu}$, \tilde{T}_c , $\tilde{\mu}_c$, where $\tilde{k} \equiv r_0^{-1}k$, are functions of only two parameters: the "dimensionless coupling constant" \tilde{g} $\equiv (\varepsilon_0 r_0)^{-1} \times g$ and the number of fermions in a sphere of radius r_0 : $\tilde{n} = (4\pi/3)r_0^3 \times n$.

III. GROUND STATE

The kernel $K_{l'}(|\mathbf{k}|, |\mathbf{k}'|)$ in Eq. (1) is given by

$$
K_{l}(|\mathbf{k}|,|\mathbf{k}'|) = -g4\pi r_0^2(-1)^l j_{l}(|\mathbf{k}|r_0) j_{l}(|\mathbf{k}'|r_0). \quad (8)
$$

Thus, although evidently the δ -shell potential is central and therefore not separable in the sense of the NSR potential, it can be written as a sum of separable terms, each one corresponding to a different value of *l*. Accordingly the gap function $\tilde{\Delta}_{\tilde{k}}$, at the saddle point, has the following form:

$$
\widetilde{\Delta}_{\widetilde{\mathbf{k}}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \widetilde{\Delta}_{l,m} j_l(|\mathbf{k}|r_0) Y_{l,m}(\hat{\mathbf{k}}).
$$

In terms of the amplitudes $\tilde{\Delta}_{l,m}$ the usual "gap" and "density'' equations, for a homogeneous, stationary, nonpolarized state with singlet pairing ($\tilde{\Delta}_{l,m} \equiv 0$ for odd *l*), read

$$
\widetilde{\Delta}_{lm} = \sum_{l',m'} \left\{ \int \frac{d^3 \widetilde{\mathbf{k}}}{(2\pi)^3} \frac{\widetilde{g} \widetilde{\Delta}_{lm,l'm'}(\widetilde{\mathbf{k}})}{2\widetilde{E}_{\widetilde{\mathbf{k}}}} \right\} \widetilde{\Delta}_{l'm'},\qquad(9)
$$

$$
\widetilde{n} = \int \frac{d^3 \widetilde{\mathbf{k}}}{6 \pi^2} \left(1 - \frac{\widetilde{\varepsilon}_{\widetilde{\mathbf{k}}}}{\widetilde{E}_{\widetilde{\mathbf{k}}}} \right), \tag{10}
$$

FIG. 2. The strength of the attraction in the BCS limit for pairing with the first four even values of the angular momentum quantum number, $l = 0,2,4,6$.

where $\tilde{\epsilon}_{\bf k} = \tilde{\bf k}^2 - \tilde{\mu}$, $\tilde{E}_{\bf k} = \sqrt{\tilde{\epsilon}_{\bf k} + |\tilde{\Delta}_{\bf k}|^2}$ and $\tilde{\Lambda}_{lm,l'm'}(\tilde{\mathbf{k}}) \equiv (4\pi)^2 j_l(|\tilde{\mathbf{k}}|) j_{l'}(|\tilde{\mathbf{k}}|) Y^*_{lm}(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}).$

To assess the relative stability of different solutions to the self-consistency problem (9) , (10) , corresponding to the same values of \tilde{g} and \tilde{n} , one has to compare the corresponding ground-state energies:

$$
\widetilde{U} = \int \frac{d^3 \widetilde{\mathbf{k}}}{6 \pi^2} |\widetilde{\mathbf{k}}|^2 \left(1 - \frac{\widetilde{\varepsilon}_{\widetilde{\mathbf{k}}}}{\widetilde{E}_{\widetilde{\mathbf{k}}}} \right) - \sum_{l,m} \frac{|\widetilde{\Delta}_{l,m}|^2}{12 \pi \widetilde{g}} - \frac{3}{4} \widetilde{g} \widetilde{n}^2. \quad (11)
$$

Evidently Eq. (9) is an infinite system of nonlinear integral equations with, presumably, an infinite number of nontrivial solutions and there is no systematic way of finding all of them. Nevertheless, a certain subset, selected by the requirement that all but a few of the $\tilde{\Delta}_{l,m}$ be equal to zero, can be explored systematically. Since the effective coupling constant in the weak-coupling limit, Eq. (3) , is $($ for even *l* $)$

$$
K_l = -g4\pi r_0^2 j_l (k_F r_0)^2, \qquad (12)
$$

it is clear that for small \tilde{g} , and within the range of densities for which $k_F r_0 \leq 5$, we can restrict our attention to the first two values of $l=0,2$ (see Fig. 2). These are the two-body states with the lowest energy (existing at $\tilde{g} \ge 2,10$, respectively^{17,18}), and therefore this simplification is also valid for our purposes in the BE limit. Moreover, for simplicity we will consider *d*-wave states with a particular symmetry, choosing $d_{x^2-y^2}$ which has been extensively studied in other models $3,10-12,14,15$ on account of its relevance to cuprate superconductivity.³⁴

For our two trial ground states the gap function has the following form, respectively:

$$
\widetilde{\Delta}_s(\widetilde{\mathbf{k}}) \equiv \widetilde{\Delta}_s j_0(|\widetilde{\mathbf{k}}|) Y_{00},\tag{13}
$$

$$
\widetilde{\Delta}_{d_{x^2-y^2}}(\widetilde{\mathbf{k}}) = \widetilde{\Delta}_{d_{x^2-y}j_2}(|\widetilde{\mathbf{k}}|) \frac{1}{\sqrt{2}} [Y_{2,2}(\widehat{\mathbf{k}}) + Y_{2,-2}(\widehat{\mathbf{k}})].
$$
\n(14)

FIG. 3. The zeros (dashed lines) and sign ("+" and "-" symbols) of the gap function Δ_k on the (k_x, k_y) and (k_x, k_z) planes, for (a) the trial ground state with *s* symmetry and (b) the one with $d_{x^2-y^2}$ symmetry.

Note that this is a more complicated **k** dependence than that of gap functions arising from interactions of the form (2) , which depend only on the angle \hat{k} . In particular, the gap function can change sign as **k** increases in the *radial* direction of increasing $|\mathbf{k}|$, not just as the angle $\hat{\mathbf{k}}$ is varied: see Fig. 3. The oscillatory behavior as a function of $|\mathbf{k}|$ can be regarded as a direct consequence of the singling out of a particular distance by the attractive interaction (5) . More generally, we expect these oscillations, of frequency $\sim 1/r_0$, to be a generic feature of interactions that are attractive predominantly at some finite distance r_0 .

Substitution of Eq. (13) $[Eq. (14)]$ into the selfconsistency problem (9) , (10) yields a much simpler problem, which can be solved numerically for every value of \tilde{g} $\lim_{n \to \infty} \frac{1}{n}$.

For low values of \tilde{g} , we find that $\tilde{\mu} \ge \tilde{\Delta}_s$ $(\tilde{\mu} \ge \tilde{\Delta}_{d_{x^2-y^2}})$.

This is the usual weak-coupling condition⁸ characterizing the BCS limit, and consequently the numerical results display the usual generalized BCS law³⁵ $\tilde{\Delta}_s \propto \exp\{1/NK_0\}$ ($\tilde{\Delta}_{d,z_1}$ ² \propto exp{1/*NK*₂}) where *N* is the free-fermion density of states, per spin, per unit volume. To illustrate this by an example, Fig. 4 shows $\overline{\Delta}_{d_x^2-y^2}$ vs \overline{g} for constant \overline{n} = 7.5. In this regime, the nonmonotonic dependence of the effective weakcoupling constant K_l on the rescaled Fermi vector $k_F r_0$ [given in Eq. (12) ; see also Fig. 2] leads to the similarly nonmonotonic dependence of $\overline{\Delta}_s$ and $\overline{\Delta}_{d_x^2-y^2}$ on $\overline{n}=(4/9\pi)$ $\times (k_F r_0)^3$ shown in Fig. 5.³⁶

On the other hand, for large values of \tilde{g} we obtain $\tilde{\mu}$ $-\tilde{\Delta}_s$ ($\tilde{\mu} \ll -\tilde{\Delta}_{d_{\kappa^2-1}}$), which is the opposite strong-coupling condition, corresponding to the BE limit.⁸ Thus as \tilde{g} is increased, while keeping \tilde{n} constant, $\tilde{\mu}$ goes from being ap-

FIG. 4. Evolution of the amplitude of the gap function for the $d_{x^2-y^2}$ trial ground state, as a function of \tilde{g} , for fixed $\tilde{n} = 7.5$.

proximately independent of \tilde{g} , and equal to $\tilde{\varepsilon}_F$ (= the Fermi energy $\varepsilon_F = \hbar^2 k_F^2 / 2m^*$ divided by ε_0), to having the behavior

$$
\tilde{\mu} \approx \frac{\tilde{\varepsilon}_b^l}{2},\tag{15}
$$

where $\tilde{\epsilon}_b^l$ is the binding energy of the two-body bound state with angular momentum quantum number $l=0,2$ (given analytically in Refs. 17 and 18, for example), divided by ε_0 . This evolution of the chemical potential is represented in Fig. 6, for the $d_{x^2-y^2}$ trial ground state (the positive offset of μ ²/_{*p*} above $\tilde{\epsilon}_b^l/2$ that can be seen in the graph becomes very small, compared to $\tilde{\epsilon}_b^l/2$, only at larger values of \tilde{g} than those shown; additionally, it tends to zero as $\tilde{n} \rightarrow 0$).

As is well known^{7,8} the qualitative change of the ground state from BCS-like to BE-like behavior occurs when the chemical potential goes below the bottom of the band, i.e., $\tilde{\mu}$ =0. Figure 7 shows two superimposed "charts" of the crossover, for the *s* and $d_{x^2-y^2}$ ground states, obtained using this condition. The charts include also two additional boundaries for each trial ground state, corresponding to $\tilde{\mu}$ $=\Delta_s$, $\Delta_{d_{x^2-y^2}}$ and $\tilde{\mu} = -\tilde{\Delta}_s$, $-\Delta_{d_{x^2-y^2}}$, which indicate the

FIG. 5. Evolution of the amplitude of the gap function for the *s* and $d_{x^2-y^2}$ trial ground states with increasing value of \tilde{n} , for fixed $\tilde{g}=2$.

FIG. 6. Evolution of the chemical potential for the $d_{x^2-y^2}$ trial ground state, as a function of \tilde{g} , for fixed $\tilde{n} = 7.5$.

extent of the ''crossover region'' between the BCS and BE limits. These charts are very similar to the ones presented in Ref. 11 for *s*-wave pairing via the NSR and Gaussian potentials, suggesting that the density-driven crossover behavior described in that reference is generic to continuum models. The main difference that we observe for $d_{x^2-y^2}$ -wave pairing is the enlarged BCS region at low densities, due to the higher value of the coupling constant required for a two-body bound state. Interestingly, in contrast to this the charts for *s*- and $d_{x^2-y^2}$ -wave pairing seem to become quantitatively identical as \tilde{g} is increased. The oscillations of the boundary between the BCS and crossover regions at high densities are directly related to the nonmonotonic density dependence shown in Fig. 5.

Evidently, Fig. 5 suggests that at intermediate densities, at which $\tilde{\Delta}_{d_{x^2-y^2}} \gg \tilde{\Delta}_s$, the energy of the trial ground state with $l=2$ is lower than for $l=0$. The precise value of the density at which this breaking of the rotational symmetry takes place and the higher value at which the symmetry is restored are given, in the limit of small \tilde{g} , by the first two positive solutions of the following equation:

$$
j_0(\tilde{k}_F)^2 = j_2(\tilde{k}_F)^2,\tag{16}
$$

FIG. 7. ''Chart'' of the BCS to Bose crossover for the trial ground state with *s* pairing (solid lines) and the one with $d_{x^2-y^2}$ pairing (dashed lines). The thicker lines are where the chemical potential goes below the bottom of the band, while the thinner lines give an indication of the extent of the crossover region (see text).

FIG. 8. Phase diagram of the relative stability of trial ground state with *s* and $d_{x^2-y^2}$ pairing symmetry. The dashed lines indicate the position of the phase boundary in the $\tilde{g} \rightarrow 0$ limit, given by Eq. $(16).$

where $\tilde{\mathcal{K}}_F = k_F r_0$. These can be determined from Fig. 2. On the other hand, for large \tilde{g} the system is always in the BE regime, in which the energy (11) takes the form

$$
\tilde{U} = \frac{1}{2}\tilde{n}\tilde{\varepsilon}_b^l - \frac{3}{4}\tilde{g}\tilde{n}^2.
$$
 (17)

Since the Hartree term $-3/4\tilde{g}\tilde{n}^2$ is independent of *l*, at first sight this equation suggests that the $l=0$ trial ground state, for which $\tilde{\epsilon}_b^l$ is lower,⁴ must have lower energy; however, note that in general $\lim_{\delta \to 0} (\tilde{U}_s - \tilde{U}_{d_{\chi^2-y^2}}) \neq \lim_{\delta \to 0} \tilde{U}_s - \lim_{\delta \to 0} \tilde{U}_{d_{\chi^2-y^2}}$ [where \tilde{U}_s and $\tilde{U}_{d_{x^2-y^2}}$ are the energies of the two trial ground states and the limit refers to taking $\tilde{\mu} \ll -\tilde{\Delta}_s$, $-\tilde{\Delta}_{d_{x^2-y^2}}$ in Eq. (11)]. In fact there is an additional positive contribution to the energy, similar to the positive offset of the chemical potential, with respect to $\varepsilon_b^l/2$, seen in Fig. 6, which does not appear in Eq. (17) because it varies slowly with \tilde{g} and therefore becomes negligible for sufficiently large \tilde{g} (just like the offset of $\tilde{\mu}$). This repulsion is different for pairs with different internal structures, and so it is only in the $\tilde{n} \rightarrow 0$ limit which Eq. (17) allows us to conclude that the $l=0$ state is preferred at high \tilde{g} . At finite densities, the energies have to be evaluated numerically. Nevertheless, the result, shown in Fig. 8, confirms our expectations: between the two densities given by Eq. (16) the $d_{x^2-y^2}$ trial ground state is more stable, thus breaking the rotational symmetry of the system, but only for relatively small values of the coupling constant. As \overline{g} is made larger, the range of densities in which this symmetry is broken becomes progressively smaller until, above some critical value of $\tilde{g} \sim 14$, the system prefers the *s* state at all densities. Thus the region in parameter space in which the rotational symmetry is broken is relatively small. In particular, it is confined to the BCS side of the crossover diagram, i.e., $\tilde{\mu}$ > 0 everywhere inside the $d_{x^2-y^2}$ region.³⁷

IV. CRITICAL TEMPERATURE

Unlike the theory of the ground state that of the equilibrium phase at finite temperatures does not follow from the usual BCS theory when the superconducting instability corresponds to the BE condensation of ''preformed pairs'' (PP's). To describe such a situation one must go beyond the mean-field theory and include fluctuations. This is most readily done within the framework of a path integral representation of the partition function $Z^{(38,39)}$ We shall now proceed following this approach and keeping only the lowest significant corrections to the mean-field theory. Namely, we start with a Grassman path-integral representation of *Z* for the electrons, implement the usual Hubbard-Stratonovich transformation $38-40$ to a functional integral over a complex pairing field Δ , and, finally, expand the effective action for the fluctuations, $S_b[\Delta^*,\Delta]$, about the saddle point of the functional integral above T_c to quadratic (Gaussian) order.12,15,22,23,32 This is a well-tied approximation for the problem at hand³¹ and therefore suitable for studying the effects of pairing fluctuations on T_c in our particular model. In short, using Eqs. (1) and (8) to write the Hamiltonian as

$$
\hat{H} - \mu \hat{N} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} \hat{c}_{\mathbf{k},\sigma}^{\dagger} \hat{c}_{\mathbf{k},\sigma} + \sum_{l,m,\mathbf{q}} \frac{V_l}{L^3} \hat{b}_{l,m,\mathbf{q}}^{\dagger} \hat{b}_{l,m,\mathbf{q}} \qquad (18)
$$

[where L^3 is the sample volume and $V_l \equiv$ $(-1)^{l+1}g(4\pi r_0)^2$] suggests that we introduce bosonic fields $\Delta_{l,m,\mathbf{q}}(\omega_{\nu})$ conjugate to the operators

$$
\hat{b}_{l,m,\mathbf{q}}^{\dagger} \equiv \sum_{\mathbf{k}} j_l (|\mathbf{k}| r_0) Y_{l,m}(\hat{\mathbf{k}}) \hat{c}_{\mathbf{q}/2+\mathbf{k}\uparrow}^{\dagger} \hat{c}_{\mathbf{q}/2-\mathbf{k}\downarrow}^{\dagger}, \qquad (19)
$$

$$
\hat{b}_{l,m,\mathbf{q}} = \sum_{\mathbf{k}} j_l(|\mathbf{k}|r_0) Y_{l,m}^*(\hat{\mathbf{k}}) \hat{c}_{\mathbf{q}/2-\mathbf{k}\downarrow} \hat{c}_{\mathbf{q}/2+\mathbf{k}\uparrow},\qquad(20)
$$

which evidently create and annihilate, respectively, a pair with total momentum **q** and angular momentum quantum numbers l,m . As usual, the momentum and frequency dependence of the fields captures the dynamics of the bosonic degrees of freedom. The additional *l*,*m* dependence reflects the fact that our explicit interaction potential can bind pairs with different internal structures. Obviously the $\Delta_{l,m}$ of the previous section correspond to a homogeneous, stationary configuration of the fields, $\Delta_{l,m,\mathbf{q}}(\omega_p) \equiv \delta_{\mathbf{q},0}\Delta_{l,m}$.

Proceeding in the usual way^{12,15,22,23,32} we obtain

$$
S_b[\Delta^*, \Delta] = \beta \sum_{\mathbf{q}\nu} \sum_{l,l'} \sum_{m,m'} \Delta^*_{l,m,\mathbf{q}}(\omega_\nu)
$$

$$
\times \Gamma^{-1}_{l,m,l',m'}(\mathbf{q}, i\omega_\nu) \Delta_{l',m',\mathbf{q}}(\omega_\nu), \qquad (21)
$$

where the sum on l, l' extends only over values of the angular momentum quantum number with the same parity (both even or both odd), $\beta = 1/k_BT$ is the inverse temperature, and the $\omega_v = 2 \nu \pi/\beta$ are bosonic Matsubara frequencies. To further simplify the problem and facilitate the discussion of the BE limit, we follow the procedure employed by Zwerger and $\rm{co\text{-}works}^{15,22}$ to write a low-frequency, low-momentum expansion of the inverse propagator for the preformed pairs:

$$
\Gamma_{l,m,l',m'}^{-1}(\mathbf{q},i\omega_{\nu})/[d_{l}(\beta,\mu)d_{l'}(\beta,\mu)]^{1/2}
$$
\n
$$
= \left(-i\omega_{\nu} + \sum_{i=x,y,z} \frac{\hbar^{2}\mathbf{q}_{i}^{2}}{2m_{l,m,l,m}^{b,ii}(\beta,\mu)} - \mu_{l}^{b}(\beta,\mu)\right)
$$
\n
$$
\times \delta_{l,l'}\delta_{m,m'} + \left(\sum_{i,j=x,y,z} \frac{\hbar^{2}\mathbf{q}_{i}\mathbf{q}_{j}}{2m_{l,m,l',m'}^{b,ij}(\beta,\mu)}\right)
$$
\n
$$
\times (1-\delta_{l,l'}\delta_{m,m'}).
$$
\n(22)

This expansion takes into account the two-body bound states leading to the formation of PP's, and so it can be used to interpolate between the BCS limit, where fluctuations can be neglected, and the Bose limit, where such states dominate. Thus after appropriate rescaling of the bosonic fields the known functions $m_{l,m,l',m'}^{b,ij}(\beta,\mu)$ and $\mu_l^b(\beta,\mu)$ play the role of effective boson masses and chemical potentials, as in Refs. 8,15,22, and 23, for example. These two functions and the rescaling factor $d_l(\beta,\mu)$ are given in the Appendix. On the other hand, in the crossover regime, Eq. (22) does not adequately describe a potentially important contribution from scattering states, 8 and thus our results in that region of parameter space must be regarded simply as a convenient interpolation scheme.

Note the different chemical potentials for bosons with different values of the angular momentum. Moreover, the anisotropic dispersion relation given by $m_{l,m,l',m'}^{b,ij}(\beta,\mu)$ can describe not only the ''rigid'' propagation of a boson without changing its internal state, but also changes in its internal angular momentum through the off-diagonal terms, with $l,m \neq l',m'$. However, in the BE limit, which as usual corresponds to $\mu\beta \rightarrow -\infty$, we have $m_{l,m,l',m'}^{b,ij}(\beta,\mu) \rightarrow \infty$ for $l, m \neq l', m'$, and therefore in what follows we shall ignore these off-diagonal terms \lceil for $l, m=l', m'$, on the other hand, we recover the expected behavior^{8,15,22,23}: $m_{l,m}^{b,i}(\beta,\mu)$ $\equiv m_{l,m,l,m}^{b,ii}(\beta,\mu) \rightarrow 2m^*$].

As usual, T_c is determined by the BE condensation condition $\mu_l^b(\beta,\mu) = 0$. This gives a different critical temperature for each value of *l*. On the other hand, T_c is degenerate in $m=-l, \ldots, l$, as in BCS theory.² Since the present method can only describe an instability of the normal state, our philosophy will be to compute the $l=0$ and $l=2$ critical temperatures and then take the highest of the two as the critical temperature of the system. Moreover, we will assume that, near the critical temperature, only fluctuations with the appropriate value of *l* have to be taken into account. In general, pairs with the other value of the angular momentum quantum number l' will also be present at T_c , but in a smaller number due to the lower value of their effective chemical potential, $\mu_{l'}^b(\beta,\mu) < 0$. Our approximation thus amounts to assuming that the bosonic chemical potential for these additional PP's is indeed well below zero at the superconducting instability. This is only adequate if the $l=0$ and $l=2$ critical temperatures differ considerably, which as we shall see is the case in the BE limit. Of course in the opposite, BCS limit the fluctuations can be neglected completely. Thus again this simplified scheme should serve well as an interpolation between the two limits, but one must bear in mind that the description of the intermediate, crossover regime is only schematic.

Under the above assumptions the " T_c " and "density" equations take the form

$$
\frac{1}{\tilde{g}} = (-1)^l \frac{2}{\pi} \int_0^\infty d|\tilde{\mathbf{k}}||\tilde{\mathbf{k}}|^2 j_l(|\tilde{\mathbf{k}}|)^2 \frac{1 - 2f(\tilde{\beta}\tilde{\varepsilon}_{\tilde{\mathbf{k}}})}{2\tilde{\varepsilon}_{\tilde{\mathbf{k}}}},\qquad(23)
$$

$$
\widetilde{n} = \widetilde{n}_0 + \sum_m \delta \widetilde{n}_{l,m},\tag{24}
$$

where $\tilde{n}_0 = (4/3\pi) \int_0^\infty d|\mathbf{\vec{k}}| |\mathbf{\vec{k}}|^2 f(\tilde{\beta} \tilde{\epsilon}_{\tilde{k}})$ is the density of fermions that are unpaired above T_c and the additional contribution coming from Gaussian fluctuations is made up of terms of the form

$$
\delta \tilde{n}_{l,m} = \frac{4}{3\pi} \int_0^\infty d|\tilde{\mathbf{q}}||\tilde{\mathbf{q}}|^2 g\left(\tilde{\boldsymbol{\beta}} \frac{|\tilde{\mathbf{q}}|^2}{2}\right) \tilde{w}(|\tilde{\mathbf{q}}|),\tag{25}
$$

which correspond to fermions bound in PP's with angular momentum given by *l*,*m*. The notations $f(x)$ and $g(x)$ have been used for the Fermi and Bose distributions functions, respectively. The "weight" $\tilde{w}(\tilde{q})$ is given by

$$
\widetilde{w}(|\widetilde{\mathbf{q}}|) \equiv \left(\prod_{i=1}^{3} \widetilde{m}_{l,m}^{b,i}\right)^{1/2} \times \left[1 + \frac{1}{\widetilde{d}_{l}} \left(\frac{\widetilde{d}_{l}^{\prime}}{\widetilde{d}_{l}} \widetilde{\lambda}_{l} - \widetilde{\lambda}_{l}^{\prime}\right) \times \frac{1}{3} \left(\sum_{i} \kappa_{l,m}^{i} \widetilde{m}_{l,m}^{b,i}\right) \frac{|\widetilde{\mathbf{q}}|^{2}}{2}\right],
$$
\n(26)

where the dimensionless function $\tilde{\lambda}_l(\tilde{\beta}, \tilde{\mu})$ and the factor $\kappa_{l,m}^i$ are defined in the Appendix and each "primed" represents differentiation with respect to μ . This weight becomes unity in the BE limit $\mu\beta\rightarrow-\infty$, corresponding to bosons of mass 2*m** each.

Numerical solution of the self-consistency equations (23) and (24) for $\tilde{\beta}$ and $\tilde{\mu}$, at the relatively low value of the density \tilde{n} = 0.5, shows the expected^{8,15,22,23} smooth evolution between the BCS and BE limits, analogous to the one seen in the ground state: see Fig. 9. In particular, we find that the critical temperature for angular momentum quantum number *l* is

$$
\widetilde{T}_c^l \propto \exp\{1/NK_l\} \tag{27}
$$

for small \tilde{g} but saturates to a constant value given by

$$
k_B T_c \approx 3.315 \frac{\hbar^2}{2m^*} \left[\frac{n}{2(2l+1)} \right]^{2/3} \tag{28}
$$

in the large- \tilde{g} limit. This asymptotic behavior follows quite generally from the self-consistency equations (23) and (24) .

FIG. 9. The critical temperature for an instability to a superconducting state with $l=0$ (solid line) and $l=2$ (dashed line), as a function of \tilde{g} , for fixed $\tilde{n} = 0.5$. The increasing dotted lines are obtained by neglecting the contribution of Gaussian fluctuations to the total density, i.e., the second term on the right-hand side of Eq. (24) , while the constant dotted lines are the BE condensation temperature given in Eq. (28) .

Notably, Eq. (28) differs from the standard result (4) in the presence of the degeneracy factor $1/(2l+1)$ multiplying the density of bosons *n*/2. For an instability to an *s*-wave superconducting state, with $l=0$, Eq. (28) reduces to Eq. (4) and thus our result for the DSM coincides with those obtained earlier for models featuring the NSR (Ref. 8) and contact^{22,23,26} potentials. On the other hand, the degeneracy of the $l=2$ bound state means that, at T_c , five Bose gases condense simultaneously, but independently, leading to a much lower critical temperature. This is in contrast with the result for the anisotropic potential of Ref. 15. On the basis of this we conclude that the $l=0$ state always has higher critical temperature in the BE limit.

On the other hand, for small values of \tilde{g} (\sim 3.5) we find a nonmonotonic density dependence of the *s*- and *d*-wave critical temperatures similar to the one that we described for the amplitude of the gap function in the respective trial ground states: see Fig. 10. In particular, note that there is an intermediate range of densities for which the *d*-wave critical temperature is the highest.

FIG. 10. The critical temperature for an instability to a superconducting state with $l=0$ (solid line) and $l=2$ (dashed line), as a function of \tilde{n} , for fixed $\tilde{g} = 3.5$. The dotted lines represent the BE condensation temperatures given by Eq. (28).

FIG. 11. The fraction of fermions that are bound into PP's just above T_c for an instability to a superconducting state with $l=0$ (solid line) and *l* = 2 (dashed line), as a function of \tilde{g} , at the density of Fig. 9.

As expected, $8,15,22$ the evolution from the BCS to the Bose limits is also evidenced in the fraction of fermions that are bound in PP's just above T_c $\delta n/n$ (with $\delta \tilde{n} = \sum_m \delta \tilde{n}_{l,m}$), and in the effective mass of such PP's, $m_{l,m}^{b,i}$ (see Figs. 11 and 12, respectively): both are negligible for small \tilde{g} , while in the large- \tilde{g} limit we have $\delta n \approx n$ and $m_{l,m}^{b,i} \approx 2m^*$.

Like any theory based on a Gaussian expansion, the present one displays a nonmonotonic behavior of the critical temperature as a function of \tilde{g} in the intermediate regime (see Fig. 9). Such an enhancement^{8,22,23} is not present²⁷ in the self-consistent theory²⁶ due to Haussmann, suggesting that it is an artifact. It can be understood in terms of Eq. (28) and Fig. 12 as a result of the PP's getting lighter $(m_{l,m}^{b,i})$ $\leq 2m^*$) as the value of \tilde{g} is reduced. In the self-consistent theory, at least for a model based on the contact potential, repulsive interactions between the PP's overcompensate for this, leading to a monotonic dependence of T_c on the coupling constant²⁷ (for a more advanced treatment of these re-

FIG. 12. The effective mass of the PP's existing just above T_c for an instability to a superconducting state with $l=0$ (solid line) and $l=2$ (dashed line), as a function of \tilde{g} , for the density of Fig. 9. For the case of an instability to a superconducting state with *l* = 2, only the heaviest and lightest of the masses $m_{l,m}^{b,i}$ (corresponding to $i=z$ and $|m|=2$ and 0, respectively) have been plotted.

FIG. 13. The critical value of the chemical potential for an instability to a superconducting state with $l=0$ (*s*-wave, solid line) and $l=2$ (*d*-wave, dashed line), as a function of \tilde{g} , for fixed \tilde{n} = 0.5. The dotted lines indicate the Fermi energy $\tilde{\epsilon}_F$ and the twobody binding energies per particle $\tilde{\epsilon}_b^l/2$.

pulsive forces see Ref. 41; alternative methods to describe phase fluctuations and strong pairing correlations in superconductors are described in Refs. 42 and 13). Such interactions are completely neglected in the present treatment as is evidenced, for example, in Fig. 13 which shows the evolution of the chemical potential, lacking a positive offset like the one we found in the ground state (compare the $l=2$) curve of Fig. 13 to Fig. 6). Moreover, the description of the Gaussian fluctuations afforded by Eq. (22) turns out to be valid only for densities below the first maximum of \tilde{T}_c , as a function of \tilde{n} . At the maximum, the mass of the PP's [given] in Eq. (A9), below] becomes negative, thus making $\delta \tilde{n}$ diverge. The present treatment is therefore only valid at small values of the coupling constant, for which the fluctuations can be neglected (as in Fig. 10: the only part of the plot that shows a significant contribution from fluctuations is at denshows a significant controduon from increasingly is at defi-
sities well below the first maximum of \tilde{T}_c) or at low densities, which are below the first maximum for all sizable values of \tilde{g} (as in Fig. 9).

V. CONCLUSIONS

We have studied exotic pairing in the context of a simple model featuring fermions in a continuum with an explicit, nonretarded, central interaction potential $V(r)$: the δ -shell model. Its novel feature is that the interaction is attractive only at some finite distance r_0 . Because of this, it provides, to our knowledge, the first explicit example of BCS pairing with angular momentum quantum number $l > 0$ via a spherically symmetric (central) attraction. By using a standard functional integral approach, we have studied this breaking of the rotational symmetry in relation to the BCS to Bose crossover.

By considering two trial ground states, with *s* and $d_{x^2-y^2}$ symmetries, we have found that *the ground state with broken rotational symmetry is separated from the BE regime by a quantum phase transition*, in which the symmetry of the superconducting order parameter is increased. This is due to the higher *energy* of two-body bound states with $l > 0$, and so it can be extrapolated to any central interaction potential. More generally, for other models (such as those in which the single-particle dispersion relation and the interaction potential are anisotropic), our analysis suggests that a two-body ground state with $d_{x^2-y^2}$ symmetry is required in order for pairing to take that form in the BE regime. Such scenario is realized, for example, in a lattice model with nearestneighbor (NN) attraction and large next-nearest-neighbor (NNN) hopping.⁴³

Similarly, the critical temperature for superconductivity with angular momentum quantum number $l=0$ is found to be higher than for $l=2$ in the BE limit (of strong coupling and low densities). However, interestingly, this is due not to the higher energy, but to the related higher *degeneracy* of the two-body bound state with $l=2$. Thus together these two observations place severe constraints on any interaction potential $V(\mathbf{r})$ leading to pairing with $l > 0$ in the BE limit.

In our model, the rotational symmetry breaking is a direct consequence of a nonmonotonic dependence of the superconducting properties on the fermion density which is present only in the BCS regime. Such rise and falls can be understood in terms of the oscillatory form of the ''gap function" in **k** space, whose frequency is $\sim r_0^{-1}$, and presumably they are generic to interaction potentials that are attractive predominantly at a finite distance. In Refs. 19 and 44 the possible implications of our model to cuprate superconductors, on the basis of the similar behavior observed in the doping dependence of the superconducting gap and the critical temperature, were discussed. A similar rise and fall has been known for some time in nuclei (see Ref. 45, for example). Of particular interest, in connection with recent theoretical speculations on superfluidity in magnetically trapped gases of fermionic atoms $46-49$ (for an informal review and further references see Ref. 50), is the possibility that the present mechanism would lead to exotic pairing for sufficiently high densities in these systems. Interestingly, because the change from *s*- to *d*-wave pairing is a quantum phase transition, it can take place at arbitrarily low temperatures. On the other hand, the density would have to be raised until $r_s \sim r_0$ (where, in order to achieve a phenomenological description of the interatomic potential, r_0 may be taken to be roughly the size of a diatomic molecule).

In relation to possible future work, we end by noting that we have described the ground state of the DSM in terms of a homogeneous saddle point, and we have only taken into account pairing fluctuations around that saddle point. In principle, by performing a more general Hubbard-Stratonovich transformation, including additional fields associated with the density (not just the pairing amplitude), one could study the effect of density fluctuations as well as the possibility of phase separation through a first-order gas-liquid phase transition: physically, one expects that the attraction at a *finite* distance could favor, in addition to the pairing with $l > 0$ which we have considered here, the formation of clusters of more than two particles (as in lattice models with nearestneighbor attraction⁵¹ and unlike those with on-site attraction⁸; for a discussion of the similar phenomenon of "quartetting" see Ref. 52; see also footnote 19 of Ref. 41). Evidently, this would be very interesting in the light of recent discussions of inhomogeneity in cuprate superconductors.⁵³

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APPENDIX: EXPANSION OF THE INVERSE BOSONIC PROPAGATOR

The inverse bosonic propagator in Eq. (21) is given by

$$
\Gamma_{l,m,l',m'}^{-1}(\mathbf{q}, i\omega_{\nu}) = \frac{L^3}{g} \delta_{l,l'} \delta_{m,m'}
$$

$$
- \frac{1}{\beta} \sum_{n} \sum_{\mathbf{k}} i^{l'-l} \Lambda_{l,m,l',m'}(\mathbf{k})
$$

$$
\times G_0 \left(\frac{\mathbf{q}}{2} + \mathbf{k}, i\omega_n \right) G_0 \left(\frac{\mathbf{q}}{2} - \mathbf{k}, i\omega_{\nu} - i\omega_n \right),
$$

(A1)

where $G_0(\mathbf{k}, i\omega_n) \equiv (i\omega_n - \varepsilon_\mathbf{k})^{-1}$ (with $\varepsilon_\mathbf{k} \equiv \varepsilon_0 \tilde{\varepsilon}_\mathbf{k}$) is the free-fermion Green's function and the $\omega_n \equiv (2n+1)\pi/\beta$ are fermionic Matsubara frequencies. The derivation, starting from Eq. (18) , is entirely analogous to that of the similar expression in Ref. 22, for example. In Ref. 23, the full frequency dependence of $\Gamma^{-1}(\mathbf{q}, i\omega_{\nu})$ was taken into account to obtain the critical temperature of a model featuring the contact potential. The procedure that we follow here^{15,22} yields the same results in the BCS and BE limits and a much simpler numerical problem in the crossover regime (where any theory based on a Gaussian expansion must be regarded as an interpolation scheme anyway). First we analytically continue the second Green's function on the right-hand side of Eq. $(A1)$ with respect to the bosonic Matsubara frequency, $G_0(\mathbf{q}/2-\mathbf{k},i\omega_v-i\omega_n)\rightarrow G_0(\mathbf{q}/2-\mathbf{k},w-i\omega_n)$, and then we perform the summation over *n*. Using the contour *C* in Fig. 14 (which we deform into C_1 and C_2) we obtain

$$
\Gamma_{l,m,l',m'}^{-1}(\mathbf{q},w) = \frac{L^3}{g} \delta_{l,l'} \delta_{m,m'} - \sum_{\mathbf{k}} i^{l'-l} \Lambda_{l,m,l',m'}(\mathbf{k})
$$

$$
\times \frac{1 - f(\beta \varepsilon_{\mathbf{q}/2+\mathbf{k}}) - f(\beta[\varepsilon_{\mathbf{q}/2-\mathbf{k}}-w])}{\varepsilon_{\mathbf{q}/2+\mathbf{k}} + \varepsilon_{\mathbf{q}/2-\mathbf{k}}-w}.
$$
(A2)

It is now easy to write a low-frequency, low-momentum expansion of the form

FIG. 14. The contours used to perform the summation over the fermionic Matsubara frequencies ω_n in Eq. (A1).

$$
\Gamma^{-1}_{l,m,l',m'}(\mathbf{q}, i\omega_{\nu}) \approx a_{l,m,l',m'}(\beta, \mu) - id_{l,m,l',m'}(\beta, \mu) \omega_{\nu} + \sum_{i,j=x,y,z} \frac{\hbar^2}{2m^*} c^{i,j}_{l,m,l',m'}(\beta, \mu) \mathbf{q}_i \mathbf{q}_j
$$
\n(A3)

by simply differentiating with respect to **q** and *w*. ⁵⁴ We find that the coefficients $a_{l,m,l',m'}$ and $d_{l,m,l',m'}$ are diagonal in *m*: $a_{l,m,l',m'}(\beta,\mu)$ *l*,*m* and degenerate in *m*: $a_{l,m,l',m'}(\beta,\mu)$ $=a_l(\beta,\mu)\delta_{l,l} \delta_{m,m'}$ $\delta_{m,m'}$ and $d_{l,m,l',m'}(\beta,\mu)$ $d_l(\beta,\mu) \delta_{l,l}, \delta_{m,m'}$. The dimensionless functions $\tilde{a}_l(\tilde{\beta},\tilde{\mu})$ $\vec{a}_I(\vec{p},\vec{p},\vec{p})$ and $\vec{a}_I(\vec{p},\vec{\mu}) \equiv r_0 \epsilon_0^2 L^{-3} d_I(\vec{p},\vec{\mu})$ are given by

$$
\widetilde{a}_{l}(\widetilde{\beta},\widetilde{\mu}) = \frac{1}{\widetilde{g}} - (-1)^{l} \frac{2}{\pi} \int_{0}^{\infty} d|\widetilde{\mathbf{k}}||\widetilde{\mathbf{k}}|^{2} j_{l}(|\widetilde{\mathbf{k}}|)^{2} \frac{1 - 2f(\widetilde{\beta}\widetilde{\varepsilon}_{\widetilde{\mathbf{k}}})}{2\widetilde{\varepsilon}_{\widetilde{\mathbf{k}}}},\tag{A4}
$$

$$
\widetilde{d}_{l}(\widetilde{\beta}, \widetilde{\mu}) = (-1)^{l} \frac{2}{\pi} \int_{0}^{\infty} d|\widetilde{\mathbf{k}}||\widetilde{\mathbf{k}}|^{2} j_{l}(|\widetilde{\mathbf{k}}|)^{2}
$$

$$
\times \left\{ \frac{1 - 2f(\widetilde{\beta}\widetilde{\varepsilon}_{\widetilde{\mathbf{k}}})}{4\widetilde{\varepsilon}_{\widetilde{\mathbf{k}}}} + \frac{\widetilde{\beta}f'(\widetilde{\beta}\widetilde{\varepsilon}_{\widetilde{\mathbf{k}}})}{2\widetilde{\varepsilon}_{\widetilde{\mathbf{k}}}} \right\}, \quad (A5)
$$

where we have used the notation $f'(x) \equiv df(x)/dx$ and the dimensionless inverse temperature is $\tilde{\beta} = \varepsilon_0 \beta$. The coefficient in q^2 has the form

$$
c_{l,m,l',m'}^{i,j}(\beta,\mu) = \frac{1}{2} d_l(\beta,\mu) \, \delta_{l,l'} \, \delta_{m,m'} \, \delta_{i,j} \\
+ \kappa_{l,m,l',m'}^{i,j} \lambda_{l,l'}(\beta,\mu), \qquad (A6)
$$

where $\kappa_{l,m,l',m'}^{i,j} \equiv \int_{\Sigma(1)} d^2 \mathbf{k} Y_{l,m}^*(\hat{\mathbf{k}}) \hat{\mathbf{k}}_i \hat{\mathbf{k}}_j Y_{l',m'}(\hat{\mathbf{k}})$, which can be evaluated easily by writing it in terms of the Gaunt coefficients of relativistic quantum mechanics (see Ref. 55, for example; note in particular that $\kappa_{l,m,l,m}^{i,j} = 0$ for all $i \neq j$) and, finally, $\overline{\lambda}_{l,l'}(\overline{\beta}, \overline{\mu}) \equiv r_0 \varepsilon_0 \lambda_{l,l'}(\beta, \mu)$ is given by

$$
\widetilde{\lambda}_{l,l'}(\widetilde{\beta},\widetilde{\mu}) = i^{l'-l} \frac{2}{\pi} \int_0^\infty d|\widetilde{\mathbf{k}}||\widetilde{\mathbf{k}}|^2
$$

$$
\times j_l(|\widetilde{\mathbf{k}}|)j_{l'}(|\widetilde{\mathbf{k}}|)|\widetilde{\mathbf{k}}|^2 \frac{\widetilde{\beta}^2 f''(\widetilde{\beta}\widetilde{\epsilon}_{\widetilde{\mathbf{k}}})}{2\widetilde{\epsilon}_{\widetilde{\mathbf{k}}}}.\tag{A7}
$$

The integrands of Eqs. $(A4)$, $(A5)$, and $(A7)$ have no poles on the domain of integration, and therefore are straightforward to evaluate numerically. From comparison of Eq. $(A3)$ to Eq. (22) it is evident that the masses and chemical potentials of the PP's are given by

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$$
\tilde{\mu}_l^b(\tilde{\beta}, \tilde{\mu}) = -\tilde{a}_l(\tilde{\beta}, \tilde{\mu}) / \tilde{d}_l(\tilde{\beta}, \tilde{\mu}),
$$
 (A8)

$$
\widetilde{m}_{l,m,l',m'}^{b,i,j}(\widetilde{\beta},\widetilde{\mu}) = \left[\delta_{l,l'} \delta_{m,m'} + \frac{2 \kappa_{l,m,l',m'}^{i,j} \widetilde{\lambda}_{l,l'}}{(\widetilde{d}_l \widetilde{d}_{l'})^{1/2}} \right]^{-1},
$$
\n(A9)

where we have introduced the definitions $\tilde{\mu}_l^b(\tilde{\beta}, \tilde{\mu}) \equiv \varepsilon_0^{-1} \mu_l^b(\beta, \mu)$ and \tilde{m} $_{l,m,l',m'}^{b,i,j}(\widetilde{\beta}, \widetilde{\mu})$ $\equiv (2m^*)^{-1} m_{l,m,l',m'}^{b,i,j}(\beta,\mu)$ and we have omitted the dependence of some of the functions defined above on $\tilde{\beta}, \tilde{\mu}$ for brevity.

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- 37 Note that the fact that the phase transition at these quantum critical points is of first order is due to our choice of trial ground states, Eqs. (13) and (14) . Had we allowed for mixing of the *s* and $d_{x^2-y^2}$ order parameters, we would presumably have found two second-order (instead of one first-order) phase transitions, in analogy with the similar results in Ref. 12. Clearly, such more elaborate variational calculation would be a necessary first step for an analysis of the critical behavior at these points.
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- 54 Note that Eq. (A2) does not coincide with the similar expression in Ref. 23, obtained by analytical continuation of the inverse bosonic propagator: $\Gamma^{-1}_{l,m,l',m'}(\mathbf{q},i\omega_v) \to \Gamma^{-1}_{l,m,l',m'}(\mathbf{q},w)$. Apart from the model-specific features, which are our main concern here, it differs also in the presence of the continuous variable *w* in the argument of one of the Fermi distribution functions. At the bosonic Matsubara frequencies $w=i\omega_v$, we can write $f(\beta[\epsilon_{\mathbf{q}/2-\mathbf{k}}-i\omega_{\nu}])=f(\beta\epsilon_{\mathbf{q}/2-\mathbf{k}})$ and therefore both expressions are identical when the full frequency dependence of $\Gamma^{-1}_{l,m,l',m'}(\mathbf{q},i\omega_\nu)$ is taken into account. However, the expression in Ref. 23 does not admit a small-frequency expansion of the form $(A3)$ because as is well known $(Refs. 8 and 31)$ it has a branch cut along the real axis that crosses the imaginary axis whenever μ > 0. (On the other hand, such an expression is the correct starting point for the derivation of a time-dependent Ginzburg-Landau theory (Ref. 23), which obviously involves an expansion along the *real* axis.)
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