Transition to the Fulde-Ferrel-Larkin-Ovchinnikov planar phase: A quasiclassical investigation with Fourier expansion

R. Combescot and C. Mora

Laboratoire de Physique Statistique, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France $(Received 18 November 2004; published 29 April 2005)$

We explore, in three spatial dimensions, the transition from the normal state to the Fulde-Ferrel-Larkin-Ovchinnikov superfluid phases. We restrict ourselves to the case of the "planar" phase, where the order parameter depends only on a single spatial coordinate. We first show that, in the case of the simple Fulde-Ferrell phase, singularities occur at zero temperature in the free energy which prevents, at low temperature, a reliable use of an expansion in powers of the order parameter. We then introduce in the quasiclassical equations a Fourier expansion for the order parameter and the Green's functions, and we show that it converges quite rapidly to the exact solution. We finally implement numerically this method and find results in excellent agreement with the earlier work of Matsuo *et al.* In particular, when the temperature is lowered from the tricritical point, the transition switches from first to second order. In the case of the first-order transition, the spatial dependence of the order parameter at the transition is found to be always very nearly a pure cosine, although the maximum of its modulus may be comparable to the one of the uniform BCS phase.

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I. INTRODUCTION

Despite being actively investigated for 40 years the problem of the structure of the superconducting order parameter in very high fields is still the subject of intensive research. In the compounds of interest the coupling of the magnetic field to electronic spins can no longer be ignored, and the situation where it is the only relevant one has to be considered. In this case one faces the problem of pairing electrons, for which the spin up and spin down chemical potentials are not the same. This question has been addressed independently by Fulde and Ferrell¹ (FF) and by Larkin and Ovchinnikov² (LO), who proposed that the best order parameter corresponds to pairs formed with a nonzero total momentum, in contrast to the standard situation of the BCS theory. It is worth noting that this kind of problem has been found recently to be quite relevant for ultracold atomic Fermi gases³ as well as for the physics of neutron stars. $4-6$ More specifically, Larkin and Ovchinnikov² considered for the order parameter superpositions of different plane waves, corresponding physically to different pair total momentum. They investigated which superposition was favored near the transition at *T*=0. Nevertheless they considered only a secondorder phase transition, which is not the most general situation as we will discuss below. Moreover, in addition to the "crystalline" states that they investigated, there are other possible states. For example, it has been found by Shimahara⁷ that a "cylindrical" state, made by a superposition of plane waves with orientation in all possible directions within a plane, is favored for a second-order phase transition compared to the "crystalline" structures investigated by LO. Similarly in a two-dimensional situation, Shimahara⁸ has shown that it is favorable to increase the number of plane waves as the temperature is lowered. Very recently we have shown in the same two-dimensional situation 9 that, when the temperature goes to zero, the complexity of the order parameter further increases with a cascade of phase transitions corresponding to order parameters with larger and larger number of plane waves. Hence the question of the exact structure of the order parameter in the FFLO phases is still an open problem. Since most experiments identifying tentatively FFLO phases rest heavily on the theoretical analysis, this is also a problem with major experimental implications.

In a preceding paper¹⁰ we have investigated analytically the transition to the FFLO phases in the vicinity of the tricritical point (TCP), where the FFLO transition line starts. This point is located at $T_{\text{top}}/T_{c0}=0.561$ where T_{c0} is the critical temperature for $\bar{\mu}=0$, with $2\bar{\mu}=\mu_{\uparrow}-\mu_{\downarrow}$ being the chemical potential difference between the two fermionic populations forming pairs, as for example spin up and down electrons (the corresponding effective field is $\bar{\mu}_{\text{top}} / T_{c0}$ $=1.073$). In agreement with preceding numerical work^{11–13} we have found that the transition is first order to an order parameter which is, to a very good precision, simply proportional to a one-dimensional "planar" texture $\Delta(\mathbf{r})$ \sim cos($\mathbf{q} \cdot \mathbf{r}$). This order parameter is actually the one which has been shown by Larkin and Ovchinnikov² to be the most favorable for a (second order) transition at $T=0$. Compared with other works, we have been able to understand qualitatively and quantitatively the reasons which favor this order parameter with respect to all the other possible ones. Namely we have shown that a real order parameter is favored, and that, among these states, those with the smallest number of plane waves are preferred. This then leads to an order parameter with a $cos(\mathbf{q}_0 \cdot \mathbf{r})$ dependence, in agreement with preceding work.

A remarkable feature of the results is that the location in the $\bar{\mu}$, *T* plane of this first-order transition toward the "planar" order parameter is very near the standard FFLO secondorder phase transition. This is true not only near the TCP10–12 but also almost down to $T=0^{13}$ (actually the transition to the "planar" order parameter goes back to a second-order phase transition at low temperature in agreement with LO). This proximity of a second-order transition may lead one to believe that the order parameter Δ is reasonably small at the first-order transition. This is trivially valid near the TCP where a Landau-Ginzburg-type expansion up to sixth order in order parameter Δ could be performed,^{10,11} but it is a tempting hypothesis even at lower temperature. This possibility has been explored by Houzet *et al.*¹² They found problems in applying this scheme because, for the stablest phase, namely the planar one, the coefficient of the sixth order in Δ changes sign when the temperature is lowered not much below the TCP. This leads to an instability and so the expansion up to sixth order in powers of Δ becomes inconsistent.

We will first analyze this problem and show that it is already present in the simple case of the Fulde-Ferrell phase where the order parameter is given by $\Delta(\mathbf{r}) = \Delta \exp(i\mathbf{q} \cdot \mathbf{r})$. This analysis gives a clear hint that an expansion in powers of Δ is going to fail anyway at low temperature. This suggests that one should avoid performing such an expansion. Among the various possibilities for improving the situation, one of them is to remark that, at the transition, near the TCP, the actual order parameter is quite near a simple superposition of plane waves¹⁰ even if the transition is first order (for a second-order transition the order parameter is exactly such a superposition, as investigated, 2 for example, by Larkin and Ovchinnikov at $T=0$). So the power expansion near the TCP amounts also to keep only the lowest order in a Fourier expansion of the order parameter. This leads to look for a Fourier expansion in the equations instead of a Δ expansion.

Since we want to deal with the full nonlinear, spacedependent problem, the convenient starting point is not Gorkov's equations, but rather the quasiclassical equations of Eilenberger, 14 and Larkin and Ovchinnikov.¹⁵ Not only are those equations in their simplest form the most compact and convenient formulation of our problem, but a major advantage is that they can be extended in full generality to much more complex situations¹⁶ and allow to formulate transport problems, including many-body effects, with the same level of efficiency. However, since we have to deal with a comparatively simpler problem, we will use for simplicity in this paper the original formulation and notations of Eilenberger.¹⁴ In comparison, the general formalism is used by Burkardt and Rainer¹⁷ for an analysis of a FFLO transition in two dimensions with a planar order parameter.

In this paper we will show that the introduction of a Fourier expansion in the quasiclassical equations allows one to obtain a solution which converges very rapidly toward the exact result. As a consequence a few terms in the expansion provide an excellent approximation. Here we will just deal with the principle of this method and its application to the planar transition. In particular we will rederive the results of Matsuo *et al.*¹³ Applications to other more complex cases, which are the more fundamental interest of this procedure, will be considered in another paper.

The paper is organized as follows. In the next section we consider the free energy and study in particular the simple case of the Fulde-Ferrell phase, and show that it has singularities at $T=0$ which make an expansion in powers of the order parameter unreliable. In Sec. III we explain our Fourier expansion for the simplest case of a cosine order parameter. This is then generalized in the following section to any (onedimensional) order parameter. Finally, we give in Sec. V the results of the numerical implementation of our method.

II. THE FULDE-FERRELL PHASE *T***=0 FREE ENERGY**

We will show that the problems arising in the expansion of the free energy in powers of the order parameter are already present when one considers the simple Fulde-Ferrell (FF) state. Let us start with the completely general expression, that we will use further on, for the free energy difference per unit volume between the superconducting state and the normal state:17–19

$$
\Omega_{s} - \Omega_{n} = \int d\mathbf{r} \frac{1}{V} |\Delta(\mathbf{r})|^{2}
$$

+ $4 \pi T N_{0} \text{ Re} \sum_{n=0}^{\infty} \int_{\bar{\omega}_{n}}^{\infty} d\omega \int \frac{d\Omega_{k}}{4\pi} [g_{s}(\omega, \hat{\mathbf{k}}, \mathbf{r})$
- $g_{n}(\omega, \hat{\mathbf{k}}, \mathbf{r})].$ (1)

Here *V* is the standard BCS interaction and N_0 is the single spin density of states at the Fermi energy. The difference $\mu_{\uparrow} - \mu_{\downarrow} = 2\bar{\mu}$ between spin up and spin down chemical potentials comes in the definition of $\bar{\omega}_n = \omega_n - i \bar{\mu}$ where $\omega_n = \pi T(2n+1)$ are Matsubara frequencies. For the " ξ -integrated" or quasiclassical Green's functions we have used Eilenberger's notations $g(\omega, \mathbf{k}, \mathbf{r})$ $=(i/\pi)\int d\xi_k G(\omega, \mathbf{k}, \mathbf{r})$ where $\xi_{\mathbf{k}}$ is the kinetic energy measured from the average Fermi level $(1/2)(\mu_{\uparrow}+\mu_{\downarrow})$ and $G(\omega_n, \mathbf{k}, \mathbf{r})$ is the usual temperature Green's function [these Green's functions we deal with are those for up spin; the down spin Green's functions are obtained by a simple transform and the sum over the spin leads us to take the real part in Eq. (1)]. With these notations we have $g_n(\omega_n, \hat{\mathbf{k}}, \mathbf{r}) = 1$ for ω_n > 0. It results directly from the starting Gorkovs equations² that the Green's functions in the presence of the effective field $\bar{\mu}$ are obtained from those in the absence of it by the simple replacement of ω_n by $\bar{\omega}_n$.

We look now for the expression of this free energy at *T* $=0$ for the simple FF state where the order parameter is given by $\Delta(\mathbf{r}) = \Delta \exp(i\mathbf{q} \cdot \mathbf{r})$. Since in this case $|\Delta(\mathbf{r})|^2 = \Delta^2$, the Green's function is just obtained from the standard BCS one by shifting² all the momenta by $q/2$. Finally, the quasiclassical Green's function is just the BCS one, except that we have to change ω into $\omega - i\bar{\mu}_k$ with $\bar{\mu}_k = \bar{\mu}(1 - \bar{q}\hat{\mathbf{k}} \cdot \hat{\mathbf{q}})$, where we have defined the reduced wave vector $\overline{q} = qk_F/(2m\overline{\mu})$ (this results also from the general Eilenberger's equations we will write below).

The free energy for the standard uniform BCS phase with $\bar{\mu}$ =0 is

$$
\Omega = \Omega_s - \Omega_n = \frac{1}{2} N_0 \Delta_0^2 x^2 \ln(x^2/e),\tag{2}
$$

where $\Delta_0=2\omega_c \exp(-1/N_0V)$ is the zero temperature BCS phase gap (ω_c) is the standard cutoff of BCS theory), and we have expressed Δ in units of Δ_0 by introducing $x = \Delta/\Delta_0$. This free energy is naturally minimum for $x=1$ and the mini-

mum is $-\frac{1}{2}N_0\Delta_0^2$. In the presence of a nonzero effective field $\bar{\mu}$ > 0 this expression becomes from Eq. (1)

$$
\frac{\Omega}{N_0\Delta_0^2} = -\frac{x^2}{2} + \bar{m}^2 + \text{Re}[x^2 \ln(\bar{m} + \sqrt{\bar{m}^2 - x^2}) - \bar{m}\sqrt{\bar{m}^2 - x^2}],
$$
\n(3)

where we have also expressed $\bar{\mu}$ in units of Δ_0 by setting $m = \bar{\mu}/\Delta_0$. For $\Delta > \bar{\mu}$ this free energy reduces to $\Omega/N_0\Delta_0^2 = \frac{1}{2}x^2 \ln(x^2/e) + \overline{m}^2$ and gives the standard Clogston-Chandrasekhar^{20,21} first-order transition $\bar{m} = 1/\sqrt{2}$. On the other hand, it gives for small $\Delta \ll \bar{\mu}$ the expansion $\Omega/N_0\Delta_0^2 = x^2 \ln(2\overline{m}) - x^4/8\overline{m}^2 - x^6/32\overline{m}^4$, leading in particular to the second-order spinodal transition for \bar{m} = 1/2. This expansion can be generalized at $T \neq 0$ as

$$
\frac{\Omega}{N_0} = \ln[T/T_{sp}(\bar{\mu}/T)]\Delta^2 + \sum_{p=1}^{\infty} (-1)^{p+1} \frac{(2p)!}{2^{2p}p!(p+1)!} A_{2p} \Delta^{2p+2}
$$
\n(4)

with

$$
A_{2p} = 2\pi T \operatorname{Re} \left(\sum_{n=0}^{\infty} \frac{1}{\bar{\omega}_n^{2p+1}} \right)
$$
 (5)

and $T_{sp}(\bar{\mu}/T)$ is the temperature of the second-order spinodal transition toward the standard BCS phase. It is interesting to note that, while the coefficients A_{2p} are clearly all positive when $\bar{\mu}$ → 0, they are given by $A_{2p} = (-1)^p / (2p\bar{\mu}^{2p})$ when *T* \rightarrow 0. Moreover, one can see that A_{2p} has *p* zeros when $\bar{\mu}/T$ goes from 0 to ∞ (one goes basically from A_{2p} to A_{2p+2} by taking a double derivative with respect to $\overline{\mu}$). Hence the higher order coefficients have many changes of sign in the low temperature range. This feature corresponds to the singular behavior which occurs for $\Delta = \bar{\mu}$ at $T=0$ in Eq. (3). It allows also us to understand that the changes of signs found by Houzet *et al.*¹² are not simple accidents, but a systematic behavior linked to the singularity appearing at *T*=0.

Finally, the *T*=0 free energy of the FF phase is obtained by replacing in Eq. (3) $\bar{\mu}$ by $\bar{\mu}_k = \bar{\mu} (1 - \bar{q} \hat{\mathbf{k}} \cdot \hat{\mathbf{q}})$ and averaging over the direction $\hat{\mathbf{k}}$ as in Eq. (1). We give the result only in the case where \bar{q} > 1 since this is the range of wave vector corresponding to the actual minimum of the free energy. One finds

$$
\frac{\Omega}{N_0 \Delta_0^2} = -\frac{x^2}{2} + \overline{m}^2 \left(1 + \frac{\overline{q}^2}{3} \right) + \frac{x^2}{2m\overline{q}} \operatorname{Re} [\overline{m}_+ \ln(\overline{m}_+ + \sqrt{\overline{m}_+^2 - x^2}) - \sqrt{\overline{m}_+^2 - x^2} + (\overline{m}_+ \to \overline{m}_-)] - \frac{1}{6m\overline{q}} \operatorname{Re} [(\overline{m}_+^2 - x^2)^{3/2} + (\overline{m}_+ \to \overline{m}_-)] , \qquad (6)
$$

where we have used the notation $\bar{m}_{\pm} \equiv \bar{m}(\bar{q} \pm 1)$.

This result has singularities for $\Delta = \bar{\mu}(\bar{q} \pm 1)$. These are just the manifestation of the singularity found in Eq. (3) for $\Delta = \bar{\mu}$, corresponding to the upper and lower bounds in the angular integration. In particular, the singularity at Δ $=$ $\bar{\mu}(\bar{q}-1)$ gives the radius of convergence of the expansion

in powers of Δ . A particular consequence is that no expansion is possible for \bar{q} =1. This is just the situation that is found when one works in a two-dimensional space. This singular situation leads to a cascade involving an infinite number of phase transitions when the temperature goes to zero, as we have shown elsewhere. 9 In the case of a threedimensional space, with which we deal in this paper, the radius of convergence is nonzero, but it is fairly small since the minimum free energy is found at low temperature for values of \bar{q} not far from the *T*=0 LO result \bar{q} =1.2. Therefore a rapidly convergent expansion for the free energy is only valid for quite small Δ , and this happens to be in contradiction with the values of Δ needed to minimize this free energy. Naturally this expansion of Eq. (6) can be performed explicitly and the problem with the convergence is then quite obvious.

Now it is clear that these same problems arise if, instead of a phase with a single plane-wave as is the FF phase, we consider a more complicated phase which is a sum of plane waves, such as the planar phase $\Delta(\mathbf{r}) \sim \cos(\mathbf{q} \cdot \mathbf{r})$. This is already obvious from the fact that the terms which arise in the expansion for the FF phase will also appear in the expansion for this phase. Other terms with weaker singularities at Δ $=$ $\bar{\mu}(\bar{q}-1)$ will also be present. We note that a singularity is already present in the fourth-order terms investigated² by LO, as it can be seen from the explicit expression of their integral J, but it occurs for a specific value of the angle between the wave vectors, which happens to be irrelevant for their final conclusion. Therefore we come to the conclusion that, due to the singular behavior which occurs at $T=0$, we cannot rely anymore on an expansion in powers of Δ when the temperature is lowered. It is conceivable that such an expansion could still be proper by accident for a specific phase, but it is unsafe for a general exploration of the various phases in competition. A possible partial cure for this problem could be to sum up the most divergent contributions, which are precisely those occuring in the FF phase. We have tried such an approach, but, although it provides some improvement, it clearly does not lead to a satisfactory situation.

Therefore, in an attempt to extend the simple approach around the TCP, we will in the next section proceed to a Fourier expansion in the exact quasiclassical formulation of the problem. This will prove to be completely satisfactory.

III. FOURIER EXPANSION

We start from Eilenberger's equations for the diagonal $g(\omega, \hat{\mathbf{k}}, \mathbf{r})$ and off-diagonal $f(\omega, \hat{\mathbf{k}}, \mathbf{r})$ quasiclassical propagators, which we simplify from the outset by taking $\hbar = 1$ and $m=1/2$. They read¹⁴

$$
(\omega + \mathbf{k} \cdot \nabla) f(\omega, \hat{\mathbf{k}}, \mathbf{r}) = \Delta(\mathbf{r}) g(\omega, \hat{\mathbf{k}}, \mathbf{r}),
$$

$$
(\omega - \mathbf{k} \cdot \nabla) f^{+}(\omega, \hat{\mathbf{k}}, \mathbf{r}) = \Delta^{*}(\mathbf{r}) g(\omega, \hat{\mathbf{k}}, \mathbf{r}),
$$

$$
2\mathbf{k} \cdot \nabla g(\omega, \hat{\mathbf{k}}, \mathbf{r}) = \Delta^{*}(\mathbf{r}) f(\omega, \hat{\mathbf{k}}, \mathbf{r}) - \Delta(\mathbf{r}) f^{+}(\omega, \hat{\mathbf{k}}, \mathbf{r}), \quad (7)
$$

where **k** is at the Fermi surface $k = k_F$. Actually *g* is given in terms of f and f^+ by the normalization condition:

$$
g(\omega, \hat{\mathbf{k}}, \mathbf{r}) = [1 - f(\omega, \hat{\mathbf{k}}, \mathbf{r}) f^+(\omega, \hat{\mathbf{k}}, \mathbf{r})]^{1/2},
$$
 (8)

so the last equation results from the two first ones. These ones are also related 14 since

$$
f^*(-\omega, \hat{\mathbf{k}}, \mathbf{r}) = f^+(\omega, \hat{\mathbf{k}}, \mathbf{r}), \quad g^*(-\omega, \hat{\mathbf{k}}, \mathbf{r}) = -g(\omega, \hat{\mathbf{k}}, \mathbf{r}),
$$

$$
f^*(\omega, -\hat{\mathbf{k}}, \mathbf{r}) = f^+(\omega, \hat{\mathbf{k}}, \mathbf{r}), \quad g^*(\omega, -\hat{\mathbf{k}}, \mathbf{r}) = g(\omega, \hat{\mathbf{k}}, \mathbf{r}).
$$
 (9)

In this paper we consider only an order parameter that varies only along the *x* axis. Accordingly *f* and *g* depend only on this variable. Moreover, we assume that the order parameter is periodic in this direction, which is the situation occuring in the FFLO transition. We also restrict ourselves to real order parameters since these have been found to correspond to the highest critical temperature in the vicinity of the TCP, and the LO solutions are also real, so this property is expected to be widely satisfied. Anyway, the generalization to an intrinsically complex order parameter should not make many difficulties.

Then we proceed to a Fourier expansion of this order parameter. Let us first assume, in order to present our method in the simplest case, that only the lowest harmonic is relevant. This amounts to taking

$$
\Delta(x) = 2\Delta \cos(qx). \tag{10}
$$

We will consider at the end of the paper the general situation, but we will actually find that, for our problem, the actual order parameter at the transition is very nearly a simple cosine. For fixed **k** Eilenberger's equations are a set of firstorder differential equations for the variation of the Green's functions along **k**. So we take a reduced variable along this direction by setting $\mathbf{r} = \mathbf{k}X$, which gives $\mathbf{k} \cdot \nabla = d/dX$ and $\Delta(x) = 2\Delta \cos(QX)$ where we have introduced $Q = k_F q \cos \theta$ with θ the angle between **k** and the *x* axis. Then we make a Fourier expansion of the Green's functions:

$$
f(X) = \sum_{n} f_n e^{inQX}, \quad f^+(X) = \sum_{n} f_n^+ e^{inQX}, \quad g(X) = \sum_{n} g_n e^{inQX}.
$$
\n(11)

Explicit substitution of Eq. (11) in Eilenberger's equations [Eq. (7)] gives

$$
f_n = \frac{\Delta}{\omega + inQ}(g_{n-1} + g_{n+1}),
$$

\n
$$
f_n^+ = \frac{\Delta}{\omega - inQ}(g_{n-1} + g_{n+1}),
$$

\n
$$
g_n = \frac{\Delta}{2inQ}(f_{n-1} + f_{n+1} - f_{n-1}^+ - f_{n+1}^+).
$$
 (12)

The solutions of these equations have simple symmetry properties, which can be checked directly for example by generating explicitly the solution by a perturbation expansion. Actually they arise quite generally from the fact that we deal with an order parameter that is real and even (i.e., parity is not broken). This is more conveniently seen by taking the case where ω is real. However, one has to keep in mind that we will deal finally with a complex ω . Nevertheless the symmetry properties are still valid generally in this case.

For a real order parameter, $f(X)$, $f^+(X)$, and $g(X)$ are real, which is consistent with Eilenberger's equations. This implies $f_{-n} = f_n^*$, $f_{-n}^+ = f_n^{+*}$, and $g_{-n} = g_n^*$. Moreover, for an even order parameter, Eqs. (7) are unchanged when $(\hat{\mathbf{k}}, \mathbf{r})$ is changed into $(-\hat{\mathbf{k}}, -\mathbf{r})$, which shows that *f*, *f*⁺, and *g* are also unchanged. Hence from Eq. (9), $f(-X) = f^+(X)$ and $g(-X)$ $=g(X)$, which leads finally to $f_n^+=f_{-n}$ and $g_n=g_{-n}$.

It is then convenient to make explicit the relation between f_n and f_n^+ by introducing $d_n = (f_n - f_n^+) / 2i$, which gives f_n $=(i-\omega/nQ)d_n$. We have then for the two quantities g_n and d_n (which are real for real ω) the recursion relations

$$
d_n = -\frac{nQ\Delta}{\omega^2 + n^2 Q^2} (g_{n-1} + g_{n+1}),
$$

$$
g_n = \frac{\Delta}{nQ} (d_{n-1} + d_{n+1}).
$$
 (13)

It is clear from these equations that $g_n \neq 0$ only for even *n*, and $d_n \neq 0$ only for odd *n*, as it can be seen, for example, by generating the solution perturbatively. Moreover, they satisfy $g_{-n} = g_n$ and $d_{-n} = -d_n$. These equations are linear and must be supplemented by the normalization condition Eq. (8) . The $n=0$ component is enough and it provides us precisely with the spatial integral $g_0 = \int d\mathbf{r} g_s(\omega, \hat{\mathbf{k}}, \mathbf{r})$, which we need in Eq. (1) to calculate the free energy:

$$
g_0^2 = 1 - \sum_{n \neq 0} (g_n g_{-n} + f_n f_{-n}^+) = 1 - \sum_{n=1} (2g_n^2 + f_n^2 + f_{-n}^2).
$$
\n(14)

 ∞

Now the interesting point is the large *n* behavior of g_n and d_n . If for example, we eliminate d_n in Eq. (13), we obtain a linear recursion relation that links g_{n+2} to g_n and g_{n-2} . Since $g_{-n} = g_n$ we have only to consider $n \ge 0$, but this becomes *n* \geq 2 when one takes into account that in Eq. (13) the relation for g_0 is identically satisfied because $d_{-1} = -d_1$. The general solution of such a recursion relation is a linear combination of two independent solutions. The large *n* behavior is found from the recursion relation, which for Δ , $|\omega| \ll |nQ|$ simplifies into $\Delta^2(g_{n+2}+g_{n-2})+n^2Q^2g_n=0$. One sees that this equation has very rapidly growing solutions satisfying $g_{n+2} \ge g_n$ $\gg g_{n-2}$ and behaving as $g_{2p+2} \sim (-1)^p (2Q/\Delta)^{2p}(p!)^2$. Naturally these solutions are not physically acceptable. On the other hand, the recursion relation has also a solution satisfying $g_{n+2} \ll g_n \ll g_{n-2}$ and behaving as $g_{2p} \sim (-1)^p (\Delta/\Delta)$ $(2Q)^{2p}(1/p!)^2$, which is the physical solution we are looking for. This solution is found only if g_0 and g_2 are related by a specific boundary condition.

The very fast decrease of g_n and d_n provides an easy way to obtain a set of approximate solutions, which moreover converges rapidly to the exact one, all the more since these are g_n^2 and d_n^2 which come in Eq. (14) for the calculation of g_0 . Since g_n and d_n are very small for large *n* we just take them to be zero beyond some fixed value. This serves as a boundary condition. Then we work backward to obtain the whole set of Fourier components and normalize them properly through the normalization condition Eq. (14) . Specifically we proceed as follows. Since the recursion relations are linear we rescale g_n and d_n in order to have convenient initial values. We set $g_n = g_0 G_n$ (which implies $G_0 = 1$) and $d_n = nQg_0D_n$ and take as initial values $G_{2N+2}=0$ and D_{2N+1} \neq 0 to be determined later. Then, starting with $p=N$, we use for decreasing values of p the following recursion obtained from Eq. (13) :

$$
G_{2p} = -G_{2p+2} - \frac{\omega^2 + (2p+1)^2 Q^2}{\Delta} D_{2p+1},
$$

$$
D_{2p-1} = \frac{1}{\Delta} \left(\frac{2p}{2p-1} G_{2p} - \frac{2p+1}{2p-1} D_{2p+1} \right).
$$
 (15)

down to G_0 . All the *G*'s and *D*'s are proportional to D_{2N+1} , which is now found by enforcing $G_0=1$. Finally Eq. (14) gives explicitly for *g*⁰

$$
g_0^{-2} = 1 + 2\sum_{p=1}^{N} G_{2p}^2 + 2\sum_{p=0}^{N} [\omega^2 - (2p+1)^2 Q^2] D_{2p+1}^2.
$$
\n(16)

When we let $N \rightarrow \infty$ this equation provides the exact result for g_0 . It is interesting to note that for these large *n* we have found that g_n is proportional to Δ^n . This makes a precise link between the expansion in powers of Δ we discussed at the beginning and the Fourier expansion we are considering now. One can see our result as corresponding to resummations of infinite series, eliminating in this way the troubles mentioned in Sec. II occuring because coefficients in the Landau-Ginzburg expansion change sign as the temperature is lowered. One finds also that in the limit of large $|\omega|$ $\gg \Delta$, |*nQ*|, where one must recover the normal state Green's functions, one has $g_{2p} \sim (-1)^p (\Delta/\omega)^{2p}$. Naturally the recursion relations Eq. (15) are very convenient and very fast for a numerical implementation and in practice the situation is not very different from having an analytical expression for $g₀$. The only practical problem is linked to the determination of the square root in obtaining g_0 from Eq. (16), but this is solved by noticing that, from the general spectral representation, one has Re $g_0 \ge 0$ when $\omega_n > 0$.

The simplest of these approximations corresponds to take *N*=0 and it is given explicitly by

$$
g_0 = \left(1 + 2\Delta^2 \frac{\omega^2 - Q^2}{(\omega^2 + Q^2)^2}\right)^{-1/2}.\tag{17}
$$

This is already a quite nontrivial approximation. Since it is correct up to order Δ^2 it gives the proper location for the standard FFLO second-order transition line. Moreover, as we will see it gives qualitatively and semiquantitatively the correct results, with a first-order transition down from the TCP which becomes a second-order transition at low temperature in agreement with Ref. 13.

Although it is quite simple, the calculation of the free energy has to be carried out numerically and naturally it is the same for all the higher order approximations. In practice it is convenient to make use in Eq. (1) of $\ln[T/T_{sp}(\bar{\mu}/T)]$ $=1/N_0V-\pi T\Sigma$ sgn $(\omega_n)/\bar{\omega}_n$ to rewrite it as

$$
\frac{\Omega_s - \Omega_n}{N_0} = \ln[T/T_{sp}(\bar{\mu}/T)] \int d\mathbf{r} |\Delta(\mathbf{r})|^2
$$

+ $4\pi T \sum_{n=0}^{\infty} \int_{\omega_n}^{\infty} d\omega \text{ Re}\left(\langle g_0(\omega - i\bar{\mu}, \hat{\mathbf{k}})\rangle_k - 1$
+ $\frac{1}{2(\omega - i\bar{\mu})^2} \int d\mathbf{r} |\Delta(\mathbf{r})|^2\right),$ (18)

where we have made no assumption on the spatial dependence of $\Delta(\mathbf{r})$. In the present case Eq. (10) gives $\int d\mathbf{r} |\Delta(\mathbf{r})|^2 = 2\Delta^2$. The form Eq. (18) is convenient for the frequency integration since the integrant behaves as ω^{-4} for large ω , with a corresponding behavior ω_n^{-3} in the Matsubara frequency summation. One may replace $\ln[T/T_{sp}(\bar{\mu}/T)]$ by $\ln[\bar{\mu}/\bar{\mu}_{sp}(\bar{\mu}/T)]$ where $\bar{\mu}_{sp}(\bar{\mu}/T)$ is the spinodal field for a given $\overline{\mu}/T$, since $\overline{\mu}_{sp}(\overline{\mu}/T)/T_{sp}(\overline{\mu}/T) = \overline{\mu}/T$. Finally the angular average amounts to an integration over *Q* since $\langle g_0(\hat{\mathbf{k}}) \rangle_k = \int (d\Omega_k/4\pi) g_0(\hat{\mathbf{k}}) = \int_0^1 du g_0(Q = \overline{\mu} \overline{q} u)$ with $u = \cos \theta$ and $\bar{q} = qk_F/\bar{\mu} \equiv \hbar qk_F/(2m\bar{\mu})$.

Since we are only interested in the transition from the normal to the FFLO state, in order to obtain the corresponding critical temperature T_c we look for the highest temperature *T* (or effective field $\bar{\mu}$) at which $\Omega_s - \Omega_n = 0$. Precisely this leads to the following equation for $T=T_c$.

$$
\ln[T/T_{sp}(\bar{\mu}/T)] = -\operatorname{Min} \frac{2\pi T}{\Delta^2} \sum_{n=0}^{\infty} \int_{\omega_n}^{\infty} d\omega \operatorname{Re} \left(\langle g_0(\omega - i\bar{\mu}, \hat{\mathbf{k}}) \rangle_k - 1 + \frac{\Delta^2}{(\omega - i\bar{\mu})^2} \right). \tag{19}
$$

Since for homogeneity the right-hand side of this equation is only a function of $T/\bar{\mu}$, $\Delta/\bar{\mu}$, and $\bar{q}/\bar{\mu}$, one has to minimize with respect to $\Delta/\bar{\mu}$ and $\bar{q}/\bar{\mu}$, at fixed $T/\bar{\mu}$.

At *T*=0 this simplifies somewhat. The summation over Matsubara frequencies goes to an integral which is performed by a by-parts integration. This gives for the critical field $\bar{\mu}$

$$
\ln[\bar{\mu}/\bar{\mu}_{sp}(T=0)] = -\operatorname{Min} \frac{1}{\Delta^2} \int_0^{\infty} d\omega \omega \operatorname{Re} \left(\langle g_0(\omega - i\bar{\mu}, \hat{\mathbf{k}}) \rangle_k - 1 + \frac{\Delta^2}{(\omega - i\bar{\mu})^2} \right). \tag{20}
$$

Finally we write down the self-consistency equation (or "gap equation") for the order parameter, which comes out quite generally when the free energy is minimized with respect to variations of this order parameter. This equation gives the necessary feedback to Eq. (7) where $\Delta(\mathbf{r})$ cannot be naturally an open function. In practice we will make little use

of it since we will rather minimize directly the free energy with respect to the order parameter. The self-consistency equation¹⁴ can be written as

$$
\Delta_n \ln[T/T_{sp}(\bar{\mu}/T)] = 2\pi T \sum_{m=0}^{\infty} \text{Re}\left(\langle f_n(\omega - i\bar{\mu}, \hat{\mathbf{k}}) \rangle_k - \frac{\Delta_n}{\omega - i\bar{\mu}} \right)
$$
(21)

by making the same transformation from T_{c0} to $T_{sp}(\bar{\mu}/T)$ as we did to find Eq. (18). In this equation Δ_n is the component in the Fourier expansion of $\Delta(\mathbf{r})$, as it is explicitly defined in Eq. (22) at the beginning of the next section.

IV. GENERAL ORDER PARAMETER

We consider now the extension of our Fourier expansion, presented in Sec. III, to a general order parameter:

$$
\Delta(x) = \sum_{n} \Delta_n e^{inQX}.
$$
 (22)

We assume again a real order parameter, which implies Δ_n^* $=\Delta_{-n}$. We also restrict ourselves as before to an order parameter even with respect to *x*, which makes Δ_n real. Substitution as above in Eilenberger's equations gives the following generalization of Eq. (12) :

$$
(\omega + inQ)f_n = (\omega - inQ)f_n^+ = \sum_{p=1}^{\infty} \Delta_p (g_{n-p} + g_{n+p}),
$$

$$
2inQg_n = \sum_{p=1}^{\infty} \Delta_p (f_{n-p} + f_{n+p} - f_{n-p}^+ - f_{n+p}^+).
$$
 (23)

Here we have also assumed for the moment that the spatial average of the order parameter is zero, that is, $\Delta_0=0$. Introducing again $d_n = (f_n - f_n^+) / 2i$, we obtain the recursion relations:

$$
d_n = -\frac{nQ}{\omega^2 + n^2 Q^2} \sum_{p=1}^{\infty} \Delta_p (g_{n-p} + g_{n+p}),
$$

$$
g_n = \frac{1}{nQ} \sum_{p=1}^{\infty} \Delta_p (d_{n-p} + d_{n+p}).
$$
 (24)

We consider now the practical situation met in numerical use of these equations. In this case the number of Fourier components for the order parameter will be finite, so we have a maximum integer *P* for which $\Delta_p = 0$ when $p > P$. We look again at the behavior of the physical solution for d_n and g_n when *n* goes to infinity, and show that it is consistent with a fast factorial type decrease, as we have found in Sec. III. Indeed in this case the dominant term in the sums found on the right-hand side of Eq. (24) is the one where d_n or g_n has the smallest index *n*, which gives $d_n \sim -\Delta_P g_{n-P}/(nQ)$ and $g_n \sim \Delta_P d_{n-P}/(nQ)$. This leads to $g_n \sim (\Delta_P/Q)^{n/P}/(n!)^{1/P}$. Although this is still a fast-factorial-type decrease, it gets slower when *P* increases. On the other hand, the large *n* behavior contains the power law dependence $(\Delta_p)^{n/P}$, where

in generic situations Δ_p is expected to be very small for large *P*. This is indeed what is found when one writes the selfconsistency equation,¹⁴ Eq. (21), which gives Δ_n in terms of f_n . This fast decrease of Δ_n corresponds to the standard situation, where there is no smaller physical length scale for $\Delta(x)$ than $1/q$ itself. However, one can think of other particular situations, where this fast decrease of Δ_n does not hold and which should be dealt with specifically. Ultimately this convergence problem has to be handled numerically by making calculations for increasing *P* and looking when reasonable convergence has been achieved. This is what we will do below with our present problem of finding the location of the transition.

Finally we make the same practical use of this fast convergence property as in Sec. III. We take as the boundary condition that g_n and d_n are zero beyond some fixed value N. This allows us to calculate all the g_n and d_n within a common multiplicative factor, which is then found by the normalization condition, Eq. (14) . *N* is progressively increased until convergence has been obtained. The situation for solving the practical problem of finding the g_n 's and the d_n 's is less convenient than in Sec. III. However, we still have a linear problem for which very efficient numerical procedures are known. We have basically to handle a matrix. Instead of having a tridiagonal matrix, with just matrix elements right below and above the main diagonal, we have now a band diagonal matrix with, in addition to the main diagonal, 2*P* diagonals with nonzero matrix elements.

To be more specific we have now to take into account that, in our problem, only odd Fourier components Δ_{2n+1} of the order parameter are nonzero. First we consider only order parameters with a zero spatial average $\Delta_0=0$, since taking a nonzero value amounts to mix in the order parameter of the uniform BCS phase, which is energetically unfavorable. Hence it is reasonable to assume that similarly a nonzero Δ_0 is unfavorable. Next we can see, for example, by an iterative treatment to all orders, in order to obtain an exact solution of Eilenberger's equations, that we have only odd components. Indeed if we start with the simple $\Delta(x)=2\Delta \cos(qx)$ that we considered in Sec. III, we generate only odd Fourier components in $f(X)$ and even components in $g(X)$ as we have seen. Now this $f(X)$ in turn generates only odd components for $\Delta(x)$ from the self-consistency equation, Eq. (21). But from Eq. (24) this is again completely compatible with only odd components for $f(X)$ and even for $g(X)$. Naturally it can also be seen directly from the starting Eilenberger's equations that such a solution is a consistent one. We note that such a solution with odd components means that, by shifting *x* by $\pi/(2q)$, we obtain an order parameter that is odd with respect to x , in the same way as it transforms Eq. (10) into $2\Delta \sin(qx)$.

Then it results from Eq. (24) that, just as in Sec. III, g_n $\neq 0$ only for even *n*, and $d_n \neq 0$ only for odd *n*. In the same way we set $g_n = g_0 G_n$ (implying $G_0 = 1$) and $d_n = nQg_0 D_n$, and we have again $G_{-n} = G_n$ and $D_{-n} = D_n$. It is now convenient to include g_n and d_n into a single unknown vector V_n , defined by $V_{2p} = G_{2p}$ and $V_{2p+1} = D_{2p+1}$. Then Eq. (24) can be merely written as $M_{mn}V_n = A_m$ with $A_n = -\Delta_n$ and the matrix *M* given by

FIG. 1. The critical temperature $T_c(\bar{\mu}/T)$ for the transition to the order parameter given by Eq. (10), divided by the FFLO critical temperature $T_{FFLO}(\bar{\mu}/T)$ obtained for the same value of $\bar{\mu}/T$. On the *x* axis, instead of $\bar{\mu}/T$, we have given $T_{FFLO}(\bar{\mu})/T_{c0}$, where T_{c0} is the maximal critical temperature, obtained for $\bar{\mu}$ =0.

$$
M_{2n,2n} = 2n,
$$

\n
$$
M_{2n+1,2n+1} = \omega^2 + (2n+1)^2 Q^2,
$$

\n
$$
M_{2m+1,2n} = \Delta_{2(m+n)+1} + \Delta_{|2(m-n)+1|},
$$

\n
$$
M_{2m,2n+1} = (2n+1)[\Delta_{2(m+n)+1} - \Delta_{|2(n-m)+1|}],
$$
\n(25)

with $m, n \geq 1$.

As explained above we truncate the infinite matrix *M* by $m, n \leq N_{\text{max}}$, which gives a matrix with finite order N_{max} . The corresponding linear equation for V_n , with $n \le N_{\text{max}}$, can be solved numerically by efficient standard routines, since as mentioned above the matrix *M* has a generalized band diagonal form. Once this is done, g_0 is still obtained from Eq. (16) , the free energy calculated from Eq. (18) and the critical temperature obtained by minimization. Finally the whole procedure is repeated for increasing values of N_{max} until convergence is achieved. In the next section we will display the corresponding numerical results.

V. NUMERICAL RESULTS

We present now the results of our numerical implementation of the above procedure. In the first susbsection below we restrict ourselves to an order parameter with only the lowest harmonic as it is given by Eq. (10) . The general case is considered afterwards.

A. Lowest harmonic

We first give in Fig. 1 the results for the calculation of the critical temperature, down from the TCP. Rather than giving $T_c(\bar{\mu})$, we cover for convenience the $(\bar{\mu}, T)$ plane in polar coordinates, rather than Cartesian coordinates, and give the critical temperature $T_c(\bar{\mu}/T)$ as a function of $\bar{\mu}/T$, equivalent to a polar angle. More precisely we plot its ratio T_c/T_{FFLO} to the FFLO critical temperature $T_{FFLO}(\bar{\mu}/T)$ obtained for the same value of the ratio $\overline{\mu}/T$. This is more suited to the

present situation since we find this ratio to be always near unity. However, to make the graph more readable, we give on the *x* axis, instead of $\bar{\mu}/T$, the value of $T_{FFLO}(\bar{\mu}/T)$ itself, compared to the standard BCS critical temperature T_{c0} , found for $\bar{\mu}=0$ (this corresponds to go along the standard FFLO transition line). Naturally when our result for T_c/T_{FFLO} goes below 1, this means that the first-order transition is less favorable than the second-order one, so when the temperature is lowered there is actually a switch from first to second order when one finds that $T_c/T_{FFLO}=1$.

We give the results of the calculation with increasing values of N_{max} going up to 6. The approximation $N_{\text{max}}=1$ corresponds to the explicit result Eq. (17) for g_0 . As already mentioned above, it is correct up to second order in Δ and consequently it gives the correct location for the FFLO transition. Moreover, we see that it gives already the proper result semiquantitatively for the order of the transition, since it gives a switch from first to second order when the temperature goes below $T_{FFLO}/T_{c0}=0.195$. The next approximation N_{max} =3 for odd N_{max} is already quite good quantitatively since it gives 0.063 for the above ratio. Full convergence is obtained for $N_{\text{max}}=5$ where we find $T_{FFLO}/T_{c0}=0.076$ in very good agreement with Matsuo *et al.*¹³ For completeness we give also in Fig. 1 our results for even N_{max} . It is less natural, from the structure of the recursion equations, to truncate them in this way. Hence it is not so surprising that the approximation $N_{\text{max}}=2$ is much worse than $N_{\text{max}}=1$ since it does not even give a switch from first to second order for the transition. Nevertheless we naturally have convergence when we increase N_{max} , and indeed we find that $N_{\text{max}}=4$ is already very good since the switch is located at $T_{FFLO}/T_{c0}=0.074$, while $N_{\text{max}}=6$ is completely converged.

A noticeable feature of Fig. 1 is that the ratio T_c/T_{FFLO} stays always very near unity, while one would have expected to find it larger since there is no obvious relation between the order parameters of the first- and second-order transitions. This behavior is also found¹⁰ near the TCP. A natural conclusion from this feature is to say that the first-order transition is actually always quite near to being a second-order one. We can check in our results if this interpretation is a coherent one by looking at the size of the order parameter (more precisely its maximal value as a function of spatial position), that is essentially the value of Δ_1 at the first order transition. If the first-order transition is nearly a second-order one, it should be small compared to a typical gap Δ_0 in the uniform BCS phase. Equivalently, in Fig. 2, we compare it to $\bar{\mu}$ since it is of order Δ_0 in all the range we are interested in (at *T* =0 the FFLO result is \bar{u} =0.754 Δ_0). Our results show clearly that the size of the order parameter at the transition is of order of the one deep in the standard BCS phase, so it is not at all possible to consider that the first-order transition is nearly a second-order one.

Finally, it is also of interest to compare the reduced wave vectors of the order parameter for our first-order transition and for the standard second-order FFLO transition. This is done in Fig. 3 where it is seen that, although there are differences, they are not very large so that the reduced wave vector is rather similar for the two transitions, in contrast with the size of the order parameter.

FIG. 2. Solid line: size of the component Δ_1 of the order parameter for the first-order transition, compared to $\bar{\mu}$, when all higher order harmonics are taken equal to zero. Dashed line: same quantity for an order parameter where Δ_3 is also non zero.

B. Higher harmonics

Naturally it is not consistent to keep only the lowest harmonic in the order parameter, as it is immediately seen from the self-consistency equation (21) . Hence we consider now the effect of higher harmonics. In a first step we have explored the effect at the transition of the inclusion of Δ_3 . We have found it quite small. This would imply normally to stop the exploration at this stage since one expects the effect of harmonics Δ_5 and higher to be even smaller. However, one might wonder whether this result is not somewhat accidental and specific to Δ_3 . This is especially a concern in the vicinity of the switching temperature from first to second order, where Δ_3 is particularly small (see Fig. 5). It could be that higher order harmonics dominate in this region, leading to a quantitative change of the first-order transition line. Hence, in order to eliminate any doubt on this question, we have explored the effect of taking Δ_5 and Δ_7 to be different from zero. Our study shows that these harmonics give also a very small contribution. Hence our conclusion is that the optimal order parameter remains always very close to a simple cosine

FIG. 3. Solid line: optimal reduced wave vector \bar{q} of the order parameter at the first order transition, for the converged solution, as a function of temperature, when only the component Δ_1 is different from zero. Long dashed line: same result when Δ_3 is also nonzero. Short dashed line: corresponding result for the second-order FFLO transition.

FIG. 4. Dashed line: critical temperature for the first-order transition for a one-dimensional order parameter form with four odd Fourier components Δ_i with $i=1, 3, 5$, and 7. Solid line: same result for the simple cosine ansatz, whereonly Δ_1 is different from zero.

in the whole temperature range from the tricritical point down to zero temperature.

Our numerical procedure is to use directly the free energy Eq. (18) by taking as an ansatz our form for the order parameter, with either three or four odd Fourier components. More precisely we maximize, with respect to \bar{q} , Δ_i with *i* $=1,3,5,7$, the critical temperature from the generalization to our case of Eq. (19) , as explained in Sec. III. We then check that our optimal form satisfies the gap equation. We have also performed calculations by making use only of the gap equation. The results are not significantly different from the ones we display below, and most of the time agree with them within numerical accuracy. From a practical point of view, we have chosen high enough values of N_{max} , typically N_{max} $=12$, so that numerical results are insensitive to changes in *N*max.

We give first in Fig. 4 our result for the critical temperature of the first-order transition. The effect of all our higher order harmonics can be only barely seen in the figure, as compared to our calculation with only the lowest harmonics Δ_1 , already given in Fig. 1.

Next we display in Fig. 5, as a function of temperature, the values of the higher order harmonics Δ_3 , Δ_5 , and Δ_7 for the optimal order parameter. It is seen that they are always quite small compared to Δ_1 . Nevertheless, around and below the switching temperature, Δ_3 and Δ_5 are of the same order while one would have rather expected Δ_5 to be small compared to Δ_3 (note that anyway these results are physically irrelevant below the switching temperature since they are for the first-order transition, while the actual transition is second order). On the other hand, Δ_7 is always negligible compared to Δ_3 and Δ_5 , except near the TCP where anyway Δ_5 and Δ_7 are essentially zero. Finally Fig. 5 shows also the results for the optimal Δ_3 and Δ_5 when $\Delta_7=0$. The difference with the preceding results is within numerical error. Similarly our result for Δ_3 when $\Delta_5 = \Delta_7 = 0$ (not shown) are also essentially indistinguishable from the result displayed in Fig. 5.

VI. CONCLUSION

In this paper we have shown that performing a Fourier expansion in the quasiclassical Eilenberger's equations pro-

FIG. 5. The optimal values for the amplitudes Δ_3 , Δ_5 , and Δ_7 in the order parameter as a function of temperature (solid lines). For comparison the results for Δ_3 and Δ_5 when $\Delta_7=0$ are also given as dashed lines.

vides a very efficient way to study the transition from the normal state to the FFLO phases in three dimensions, at least in the vicinity of the transition. We have applied this technique to the case of the transition to the one-dimensional "planar" order parameter and we have found perfect agreement with the earlier work of Matsuo *et al.* In particular we have rederived their remarkable result that, when the temperature is lowered, the transition switches from first to second order. We have shown in detail that, in the case of the first-order transition, the order parameter is nevertheless dominated by its lowest order Fourier component, in somewhat surprising contrast to what one might guess for such a transition. This feature contributes naturally to make our Fourier expansion very rapidly converging.

However, the strength of our method is not so much displayed in this case of a one-dimensional order parameter. Its major interest is rather that our approach can be fairly easily generalized to more complex order parameters, with full three-dimensional spatial dependence. As shown by Larkin and Ovchinnikov, these order parameters come in competition and, in the case of a first-order transition, it is not clear that they are not more advantageous than the standard second-order FFLO phase transition. We will indeed show, in forthcoming work, that this is the case at low temperature in three dimensions. Finally another interest of our approach is to provide some insight, even if approximate, in the analytical structure of the theory, as we have seen by providing explicit approximate analytical solutions. We believe that this might be helpful in a theoretical situation where the intrinsic nonlinearity of the equations forces mostly to purely numerical work.

- *Laboratoire associé au Centre National de la Recherche Scientifique et aux Universités Paris 6 et Paris 7.
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