Magnetic-Field-Induced Pattern of Coexisting Condensates in the Superconducting State of $CeCoIn_5$

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$CeCoIn_5$ is an anomalous superconductor which exhibits a high-magnetic-field phase that consists of a modulated magnetic coupling together with persistent superconducting order. Here we use a generic microscopic model to argue that this state is a pattern of coexisting condensates: a d-wave singlet superconducting (SC) state, a staggered π-triplet SC state, and a spin density wave (SDW). Our microscopic picture allows a calculation of the phase diagram, and physical consequences including NMR. We interpret the appearance of the SDW order in the Q phase as being induced by odd-triplet pairing.

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In usual superconductors the carriers form Cooper pairs [1] that have zero total momentum meaning that the superfluid density is homogeneous. We know for decades that it is *a priori* possible to observe at high fields the Fulde-Ferrel-Larkin-Ovchinikov (FFLO) [2] state in which the superfluid density exhibits a field dependent modulation. Among the $CeMIn_5$ class of heavy-fermion superconductors (M = Ir, Rh, Co), $CeCoIn_5$ exhibits the highest superconducting T_c at ambient pressure (2.3 K) [3]. The zero field superconducting (SC) gap symmetry is most likely of $d_{x^2-y^2}$-wave type [4]. A distinct high field superconducting (HFSC) state is observed, initially thought to be a realization of the FFLO state [5]. However, recent neutron diffraction data in the HFSC state of $CeCoIn_5$ show clearly that an almost commensurate spin density wave (SDW) at $\mathbf{Q} = (q, q, 0.5)$ develops at the onset of the HFSC region and disappears at the same upper critical field with SC in a first order transition [6]. Moreover, the modulation wave vector is not coupled to the magnitude of the external magnetic field ruling out the FFLO mechanism that produces superfluid density modulations that scale with the field. The neutron data agree well with NMR results [7–9] that reported SDW ordering in the HFSC state. Finally, in conflict with the FFLO expectations, the critical fields for entering the HFSC phase grow with temperature and this behavior becomes more pronounced as we apply pressure [10].

In this Letter we interpret these results as indicating that a novel exotic state is observed at high fields in $CeCoIn_5$ in which a pattern of coexisting condensates manifests. The specific pattern includes the d-wave singlet SC (dSC), the staggered π-triplet SC (πSC), and the SDW state. Because of particle-hole (PH) asymmetry these three condensates may either appear separately or all three together providing a new perspective on antiferromagnetic (AFM) superconductors that may include high-T_c cuprates and pnictides. We have presented these ideas for a generic situation earlier [11,12] and a similar view has been presented in work by Sigrist and co-workers [13,14] using Ginzburg-Landau and Bogoliubov–de Gennes approaches. Our work is consistent with this, but a fully microscopic theory allows a detailed connection to measurements of excitation spectra (e.g., via NMR [9]) and in principle an *ab initio* phase diagram from model parameters at the mean-field level.

The staggered πSC component has some similarity with the FFLO state in the sense that the pairs have a finite momentum and therefore the superfluid density is modulated as well. However, it is fundamentally different on basic points. First, it is a spin triplet SC state meaning that the paired quasiparticles have not antiparallel spin as in usual Cooper pairs. Second, the wave vector Q of the superfluid modulation is driven by the nesting properties of the dispersion and is common with that of the SDW modulation while in the FFLO picture the wave vector is driven by the field. Finally, the staggered πSC coexists with both dSC and SDW state, whereas the FFLO state is in fact a coexistence between singlet SC and normal state regions on different portions of the Fermi surface.

The possibility of a dynamically generated π-triplet order parameter (OP) when singlet SC coexists with SDW has already been considered [11,15]. It has been shown [11,16] that PH asymmetry is enough to induce the third OP whenever the other two are present and in this respect the three condensates form a pattern [16]. Moreover, the πSC state may also manifest in the ferromagnetic superconductor UGe_2 [17]. The spin singlet analogue of the staggered triplet OP that we report here is the so called η superconductivity [18]. Such exotic staggered states, also known as pair density waves, have been suggested to exist in underdoped cuprates [19].

Our analysis is generic, free of any model assumption, though of course in detail dependent on values of parameters which we discuss below. We consider the simplest mean-field scheme that includes the relevant OPs and the

Zeeman field:

$$\begin{aligned}\mathcal{H} = &\sum_{\mathbf{k},\alpha}\xi_{\mathbf{k}\alpha}c^{\dagger}_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha} - \sum_{\mathbf{k},\alpha,\beta}(\sigma\cdot\mathbf{n})_{\alpha\beta}M(c^{\dagger}_{\mathbf{k}\alpha}c_{\mathbf{k}+\mathbf{Q}\beta} + \text{H.c.})\\ &-\frac{1}{2}\sum_{\mathbf{k},\alpha,\beta}(\hat{\sigma}_2)_{\alpha\beta}(\Delta_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\alpha}c^{\dagger}_{-\mathbf{k}\beta} + \text{H.c.})\\ &-\frac{1}{2}\sum_{\mathbf{k},\alpha,\beta}\hat{\sigma}_2(\sigma\cdot\mathbf{n})_{\alpha\beta}(\Pi^{-\mathbf{Q}}_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}-\mathbf{Q}\alpha}c^{\dagger}_{\mathbf{k}\beta}\\ &+\Pi^{\mathbf{Q}}_{\mathbf{k}}c^{\dagger}_{\mathbf{k}+\mathbf{Q}\alpha}c^{\dagger}_{-\mathbf{k}\beta} + \text{H.c.})\\ &-\mu_B H\sum_{\mathbf{k},\alpha,\beta}(\sigma\cdot\mathbf{n})_{\alpha\beta}(c^{\dagger}_{\mathbf{k}\alpha}c_{\mathbf{k}\beta} + \text{H.c.}).\end{aligned} \tag{1}$$

Here α, β are spin indices, σ_i are Pauli matrices, and $\mathbf{n}$ is the polarization vector of the field taken parallel to that of the SDW and the staggered triplet component. The letters M, $\Delta_{\mathbf{k}}$, and $\Pi_{\mathbf{k}}$ correspond to the OPs for the SDW, dSC, and πSC, respectively. The π-triplet OP corresponds to a Cooper pair with finite momentum which equals the nesting wave vector $\mathbf{Q}$. It has the attributes $\Pi_{\mathbf{k}} = -\Pi_{\mathbf{k}+\mathbf{Q}} = \Pi^*_{\mathbf{k}} = \Pi_{-\mathbf{k}}$. Evidently, the acquired staggered momentum at commensurate $\mathbf{Q}$ allows this triplet SC OP to be of even Parity. Indeed, our d-wave singlet and staggered π-triplet SC states share the same nodal structure and therefore, their coexistence does not contradict inversion symmetry. The kinetic energy is decomposed ($\xi_{\mathbf{k}} = \delta_{\mathbf{k}} + \gamma_{\mathbf{k}}$) into a sum of periodic $\delta_{\mathbf{k}+\mathbf{Q}} = \delta_{\mathbf{k}}$ and antiperiodic $\gamma_{\mathbf{k}+\mathbf{Q}} = -\gamma_{\mathbf{k}}$ terms on $\mathbf{Q}$ translations which is also the commensurate nesting wave vector for the SDW. When $\delta_{\mathbf{k}} = 0$ there is perfect nesting and thus PH symmetry. The last term is the Zeeman Hamiltonian where we have set $\mu_B = 1$.

The orbital effect of the field is irrelevant for the phenomena that we report, and as for FFLO states, our results concern Pauli limited superconductors where orbital effects are not dominant. Note that very recently, Agterberg *et al.* elaborated a phenomenological description of the vortices for a similar state [14]. In order to treat all OPs on the same footing we use an eight component spinor that leads to an 8×8 matrix Green's function formalism treated elsewhere [11]. When the broken symmetry fields are nonzero, the excitation energies are $E_{\pm\pm}(\mathbf{k}) = H \pm [M^2 + \gamma^2_{\mathbf{k}} + \delta^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}} + \Pi^2_{\mathbf{k}} \pm 2\sqrt{(M^2 + \gamma^2_{\mathbf{k}})\delta^2_{\mathbf{k}} + 2\delta_{\mathbf{k}}M\Delta_{\mathbf{k}}\Pi_{\mathbf{k}} + (\gamma^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}})\Pi^2_{\mathbf{k}}}]^{1/2}$. Equation (1) represents a mean-field decoupling of an interacting model in the conventional way. Enforcing self-consistency leads to a system of coupled gap equations with a peculiar general structure: $\mathcal{O}^i_{\mathbf{k}} = \sum_{n,\mathbf{k}'}V^i_{\mathbf{k}\mathbf{k}'}\{\mathcal{O}^i_{\mathbf{k}'}\{\ldots\} + \delta_{\mathbf{k}'}\mathcal{O}^j_{\mathbf{k}'}\mathcal{O}^k_{\mathbf{k}'}\{\ldots\}\}$, where the n sum is on the Matsubara frequencies, i, j, k correspond to the three OPs, and $V^{i,j,k}_{\mathbf{k}\mathbf{k}'}$ are the effective pairing potentials in the respective symmetry channels. If the dispersion is PH asymmetric where $\delta_{\mathbf{k}} \neq 0$, in none of the above equations we have zero as a self-consistent solution if the other two OPs are nonzero and naturally the potentials are nonzero as well. In such a system we may either have only one or all three OPs simultaneously present. This is a generic result of relevance for all antiferromagnetic superconductors. In passing, we remark that there are numerous other patterns of different OPs that behave similarly [16]. For example, SDW, charge density wave (CDW), and ferromagnetism (FM) form a similar pattern suggested as a possible explanation for the CMR phenomenon in manganites [20].

The system of self-consistent gap equations is solved numerically on a square lattice with $\gamma_{\mathbf{k}} = -t(\cos k_x + \cos k_y)$ and $\delta_{\mathbf{k}} = -t' \cos k_x \cos k_y$ where $\mathbf{Q} = (\pi, \pi)$. This models the 2D Fermi surface of quasicylindrical sheets as revealed by de Haas–van Alphen measurements [21,22]. For convenience, separable pairing potentials of the form $V_{\mathbf{k}\mathbf{k}'} = V f_{\mathbf{k}} f_{\mathbf{k}'}$ have been used, where in our case $f_{\mathbf{k}}$ are d-wave form factors, $f_{\mathbf{k}} = \cos k_x - \cos k_y$. A thorough exploration of the combinations of potentials has been done numerically and we have found that there is a substantial parameter space where the system is a dSC in the ground state and at a sufficiently high field, remarkable transitions to a mixed phase of all three OPs are triggered. As a paradigm, we present in Fig. 1 results obtained with $V^{\text{SDW}} = V^{\text{dSC}} = V^{\pi\text{tr}} = 1.5t$ and PH asymmetry $t' = 0.35t$. At low temperatures we find two successive first order transitions with the field. The first of them is from high to smaller values of Δ. In this steplike regime the Π and the M gaps appear simultaneously. At a higher field we have the second first order transition at which all three OPs are eliminated simultaneously.

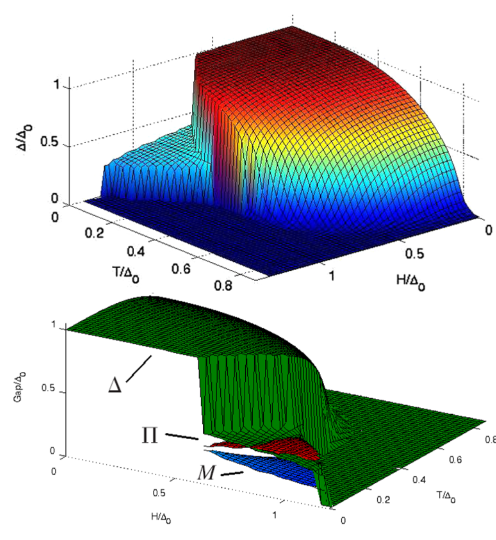

FIG. 1 (color online). The upper panel shows the field and temperature dependence of the dSC gap (Δ) when $t' = 0.35t$ normalized to its value at zero temperature and field (Δ_0). At low T, a steplike regime bounded by 1st order transitions with the field takes place. In the lower panel we plot the same as in the upper panel but for all three Order Parameters (OPs). A different orientation is chosen to highlight the existence of a low-T high field state where all three OPs coexist.

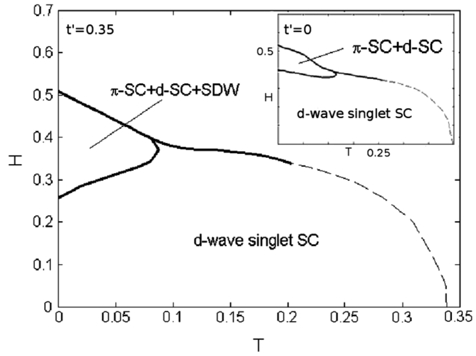

FIG. 2. Field-temperature phase diagram for a PH asymmetric system ($t' = 0.35t$) corresponding to Fig. 1. Solid lines mark 1st order and dashed lines 2nd order phase transitions. The induced SDW lies only within the boundaries of the triplet **Q**-modulated field-induced superconductivity. Some similarities with a FFLO phase diagram are evident but here the critical field for entering the multiphase state is enhanced with temperature. In the inset is shown the corresponding phase diagram in the PH symmetric case ($t' = 0$). Note that in this case there is no SDW order induced and the critical field of the steplike transition is rather temperature independent or even reduced with temperature.

The resulting H-T phase diagram is reported in the main panel of Fig. 2. The HFSC region in which the full pattern of coexisting condensates is present corresponds to the **Q** phase in $CeCoIn_5$. At the highest critical field the three OPs are simultaneously eliminated in a first order transition as observed by neutron scattering [6]. The induced SDW lies only within the boundaries of the triplet **Q**-modulated field-induced superconductivity. Some similarities with a FFLO phase diagram are evident but note the different temperature dependence of the onset of the Q phase.

It is interesting to compare to the PH symmetric case (inset of Fig. 2). Here, a similar phase diagram obtains, but SDW order is absent from the field-induced state. The SDW order is induced only because of PH asymmetry given the peculiar structure of the coupled self-consistent gap equations discussed above. Consequently, we infer that the mechanism which drives the **Q** phase in $CeCoIn_5$ is the following: to survive at the highest possible magnetic fields the d-wave singlet SC condensate, develops an even Parity, staggered in **Q** and odd in translation triplet superconducting component with the same nodal structure (i.e., the π-triplet component) with which it coexists. Particle-hole asymmetry forces the presence of the third OP, the SDW order. The full pattern of condensates appears at high fields when the dominating OP, the dSC, is ''weakened'' sufficiently by the Zeeman field. Therefore, the emergence of the pattern of condensates can be viewed as an escapeway from the formation of a magnetic quantum critical point associated with the elimination of the dominant OP. The phase diagram in the main panel of Fig. 2 corresponds to the situation in $CeCoIn_5$ [6] whereas that in the inset exhibits remarkable similarities with findings in organic superconductor κ-(BEDT-TTF)$_2$Cu(NCS)$_2$, in which a FFLO phase has also been proposed to exist [23]. The latter is thought to exhibit enhanced nesting [23], a feature which is reproduced by decreasing t' in our effective theory.

Comparing the phase diagrams in Fig. 2, we note that the coexistence ''dome'' grows with t' as shown explicitly in Fig. 3. The poles of the Green's function provide a straightforward explanation for this behavior. When $E_{--}(\mathbf{k}) = 0$ the superconductor reaches the Clogston limit [24] and the transition to the multicomponent state is triggered. For higher $\delta_{\mathbf{k}}$, smaller critical fields H_c are necessary for reaching $E_{--}(\mathbf{k}) = 0$ as confirmed by our numerical calculations. This behavior is consistent with the results of application pressure in $CeCoIn_5$ [10]—we simulate the effect of pressure as creating greater deviation from perfect nesting and therefore increased PH asymmetry $\delta_{\mathbf{k}}$.

Mean-field theories neglect fluctuation effects. For $CeCoIn_5$, the Ginzburg criterion gives $\Delta T \approx 10^{-9} T_c$ [25], validating such treatment close to T_c. On the other hand, the existence of a quantum critical point near H_{c_2} [26] implies that quantum fluctuations may play a role in the formation of the Q phase. It should be noted that in an antiferromagnetic SC, not only particle-hole but also particle-particle fluctuations in the spin channel may arise like, for example, in the cuprate YBCO [27]. Thus, within our framework, both types of quantum fluctuations appear equally important and may rise when approaching the Q phase while increasing the magnetic field. However, inclusion of such effects is out of the scope of the present Letter.

We have also calculated self-consistently the NMR Knight shift and relaxation rate as a function of temperature and field. Characteristic results are reported in Fig. 4 for the same parameters as in Fig. 1 and for three characteristic fields ($H = 0.21$, $H = 0.41$, and $H = 0.51$). At the critical temperature we observe a step in K associated with the first order transition from normal to the **Q** phase. For

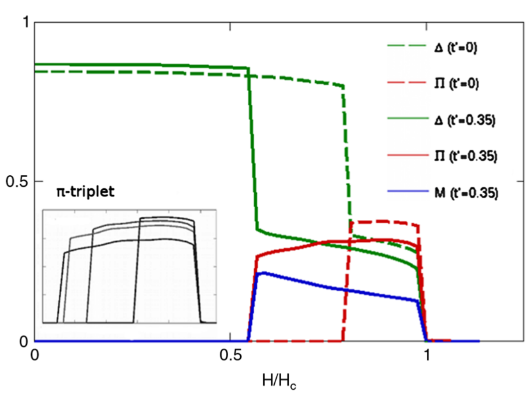

FIG. 3 (color online). Order parameter gap amplitudes as a function of the external field in the PH symmetric case $t' = 0$ (dashed lines) and in a PH asymmetric case $t' = 0.35t$ (full lines). Notice how the coexistence regime expands with t'. To illustrate this effect we plot in the inset the π-triplet gap as a function of field for $t' = (0, 0.15t, 0.25t, 0.35t)$.

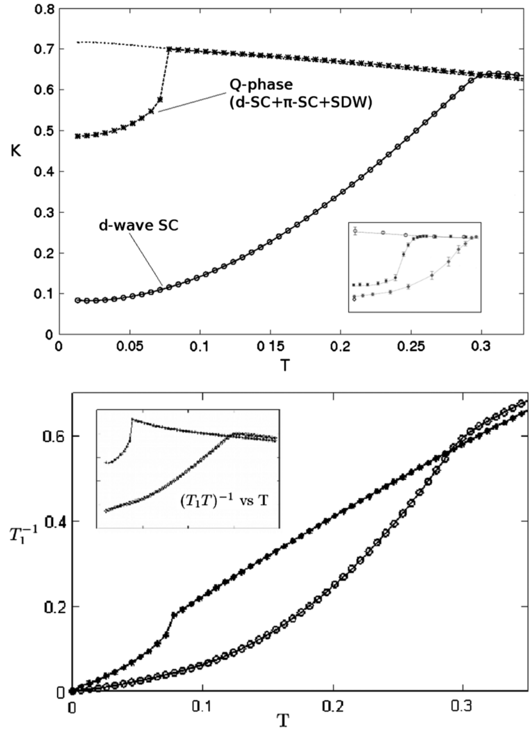

FIG. 4. Upper panel: the Knight shift K as a function of temperature for three values of the Zeeman field corresponding to different regimes in our phase diagram. For a field corresponding to the **Q** phase at low temperatures, we obtain a temperature behavior almost identical to that observed in NMR experiments [7] depicted schematically in the inset. Lower panel: the inverse NMR relaxation rate $(T_1T)^{-1}$ vs temperature for the same values of the external field that lead to the d-wave singlet and the π-triplet SC transitions as in the upper panel. In the inset $1/T_1$ vs T is shown.

even lower temperatures the susceptibility is almost constant. The zero temperature value of the knight shift is higher in the high field **Q** phase than in the dSC state (at lower fields) signaling the presence of the staggered triplet superconducting component in the **Q** phase. There is a remarkable agreement with the experimental results both for parallel [7,8] and perpendicular [9] to the ab plane field orientations, as depicted in the inset of the upper panel [7]. Here, the contribution of vortices near H_{c_2} has been neglected. However, the fact that our results describe NMR experiments for both field orientations seems to justify such an approximation.

In closing, we note that the field-induced transition to the pattern state is obtained through a generic mean-field scheme. This suggests that field-induced patterns have a generic character and should be viewed as potential alternatives to the FFLO picture not only in superconductors. Complexity in electronic matter is proven to be crucially important. For example, in CDW systems at high magnetic fields similar field-induced transitions to a CDW + SDW state [28] may occur [29], or in manganites where incommensurate charge-ordered antiferromagnetic states coexist with FM [30]. Our findings provide a new perspective in research areas as diverse as the trapped Fermi gases and situations of dense quark matter in QCD [31] where inhomogeneous condensates are very actively investigated.

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[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[2] P. Fulde and R. A. Ferrel, Phys. Rev. **135**, A550 (1964); A. I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JETP **20**, 762 (1965).
[3] C. Petrovic *et al.*, J. Phys. Condens. Matter **13**, L337 (2001).
[4] K. Izawa *et al.*, Phys. Rev. Lett. **87**, 057002 (2001).
[5] A. Bianchi *et al.*, Phys. Rev. Lett. **91**, 187004 (2003).
[6] M. Kenzelmann *et al.*, Science **321**, 1652 (2008).
[7] V. F. Mitrovíc *et al.*, Phys. Rev. Lett. **97**, 117002 (2006).
[8] B. L. Young *et al.*, Phys. Rev. Lett. **98**, 036402 (2007).
[9] J. Spehling *et al.*, Phys. Rev. Lett. **103**, 237003 (2009).
[10] C. F. Miclea *et al.*, Phys. Rev. Lett. **96**, 117001 (2006).
[11] A. Aperis *et al.*, J. Phys. Condens. Matter **20**, 434235 (2008).
[12] A. Aperis *et al.*, arXiv:0902.0553.
[13] Y. Yanase and M. Sigrist, J. Phys. Soc. Jpn. **78**, 114715 (2009).
[14] D. F. Agterberg, M. Sigrist, and H. Tsunetsugu, Phys. Rev. Lett. **102**, 207004 (2009).
[15] G. C. Psaltakis and E. W. Fenton, J. Phys. C **16**, 3913 (1983); M. Murakami and H. Fukuyama, J. Phys. Soc. Jpn. **67**, 2784 (1998); B. Kyung, Phys. Rev. B **62**, 9083 (2000); T. Maitra, H. Beck, and A. Taraphder, Eur. Phys. J. B **21**, 527 (2001); S. C. Zhang, Science **275**, 1089 (1997).
[16] S. Tsonis *et al.*, J. Phys. Condens. Matter **20**, 434234 (2008).
[17] M. Georgiou, G. Varelogiannis, and P. Thalmeier, Europhys. Lett. **82**, 67007 (2008).
[18] C. N. Yang, Phys. Rev. Lett. **63**, 2144 (1989).
[19] E. Berg *et al.*, Phys. Rev. Lett. **99**, 127003 (2007); D. F. Agterberg and H. Tsunetsugu, Nature Phys. **4**, 639 (2008).
[20] G. Varelogiannis, Phys. Rev. Lett. **85**, 4172 (2000).
[21] R. Settai, J. Phys. Condens. Matter **13**, L627 (2001).
[22] D. Hall *et al.*, Phys. Rev. B **64**, 212508 (2001).
[23] J. Singleton *et al.*, J. Phys. Condens. Matter **12**, L641 (2000).
[24] A. M. Clogston, Phys. Rev. Lett. **9**, 266 (1962).
[25] A. Bianchi *et al.*, Phys. Rev. Lett. **89**, 137002 (2002).
[26] J. Paglione *et al.*, Phys. Rev. Lett. **91**, 246405 (2003).
[27] E. Demler and S. C. Zhang, Phys. Rev. Lett. **75**, 4126 (1995).
[28] A. Aperis *et al.*, Europhys. Lett. **83**, 67008 (2008).
[29] R. D. McDonald *et al.*, Phys. Rev. Lett. **93**, 076405 (2004).
[30] G. C. Milward, M. J. Calderon, and P. B. Littlewood, Nature (London) **433**, 607 (2005).
[31] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008); R. Casalbuoni and G. Nardulli, Rev. Mod. Phys. **76**, 263 (2004).