Lifshitz Point in the Phase Diagram of Resonantly Interacting ^{6}Li-^{40}K Mixtures

K. B. Gubbels,* J. E. Baarsma, and H. T. C. Stoof

Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

(Received 10 July 2009; revised manuscript received 16 October 2009; published 3 November 2009)

We consider a strongly interacting ^{6}Li-^{40}K mixture, which is imbalanced both in the masses and the densities of the two fermionic species. At present, it is the experimentalist's favorite for reaching the superfluid regime. We construct an effective thermodynamic potential that leads to excellent agreement with Monte Carlo results for the normal state. We use it to determine the universal phase diagram of the mixture in the unitarity limit, where we find, in contrast to the mass-balanced case, the presence of a Lifshitz point. This point is characterized by the effective mass of the Cooper pairs becoming negative, which signals an instability towards a supersolid phase.

DOI: 10.1103/PhysRevLett.103.195301 PACS numbers: 67.85.−d, 03.75.Nt, 03.75.Ss, 05.30.Jp

Introduction.—Ultracold atomic Fermi mixtures are presently at the center of attention of both experimental and theoretical physicists. Because of the amazing control over this system many fundamental discoveries have been made, while more are likely to follow soon. These discoveries started with reaching the so-called BEC regime where the balanced two-component Fermi mixture turns superfluid due to the Bose-Einstein condensation (BEC) of molecules [1,2]. By using a Feshbach resonance to vary the interaction strength between atoms in different spin states, the BEC-BCS crossover between a Bose-Einstein condensate of molecules and a BCS superfluid of Cooper pairs could be directly observed [3]. Since pairing is optimal for an equal amount of atoms in each spin state and is absent for the noninteracting fully polarized system, a phase transition occurs as a function of spin imbalance [4,5]. The phase diagram of the polarized mixture was for strong interactions found to be governed by a tricritical point that resulted in the observation of phase separation [5,6]. The presence of gapless Sarma superfluidity is also likely to be present in this system [7,8], but has not been unambiguously identified yet.

Most recently, experiments have indicated that the physical consequences of yet another parameter can be explored, namely, that of a mass imbalance between the two fermionic components. A very promising mixture in this respect consists of ^{6}Li and ^{40}K, which has a mass ratio of 6.7. Several accessible Feshbach resonances are identified in the mixture [9], while both species have also been simultaneously cooled into the degenerate regime [10]. So far, experimental interest has focused on the BEC side of the Feshbach resonance, where molecules are formed. Although the mass imbalance itself does not lead to fundamental new physics here, this situation changes when the heteronuclear molecules are optically pumped to their ground state [11]. Then the molecules acquire a large electric dipole moment, which gives rise to anisotropic long-ranged interactions. In an optical lattice, this can lead to supersolid phases [12].

In this Letter we focus on a different regime, namely, the so-called unitarity limit, where the s-wave scattering length of the interspecies interaction diverges. Here, the size of the Cooper pairs is comparable to the average interparticle distance and the pairing is a many-body effect. The mass imbalance has a profound effect on the pairing now, because it strongly alters the Fermi spheres. We show that for the sufficiently large mass ratio of the ^{6}Li-^{40}K mixture, the phase diagram not only encompasses all the exciting physics known from the mass-balanced case, but is even much richer. Similar to the solely spin-imbalanced case is the presence of phase separation [13], which can occur due to the mismatch of the Fermi surfaces. Also similar is that gapless Sarma superfluidity is unstable at zero temperature [13], while there is a predicted crossover to the Sarma phase at nonzero temperatures [7]. However, the most exciting difference that we find is the presence of a Lifshitz point in the phase diagram.

At a Lifshitz point the transition to the superfluid phase undergoes a dramatic change of character. Rather than preferring a homogeneous order parameter, the system now becomes an inhomogeneous superfluid. This exotic possibility was early investigated for the weakly interacting mass-balanced case by Larkin and Ovchinnikov (LO), who considered a superfluid with a single standing-wave order parameter [14]. This is energetically more favorable than the plane-wave case studied by Fulde and Ferrell (FF) [15]. Since the LO phase results in periodic modulations of the particle densities, it is a supersolid [16]. The FF and LO phases have intrigued the physics community for many decades, but so far remained elusive in experiments with atomic Fermi mixtures. Typically, Lifshitz points are predicted at weak interactions where the critical temperatures are very low. However, in this Letter we show that the very special phase diagram of the ^{6}Li-^{40}K mixture contains both a Lifshitz and a tricritical point in the unitarity limit, as shown in Fig. 1. This is in sharp contrast to the mass-balanced case, where at unitarity a large body of theory

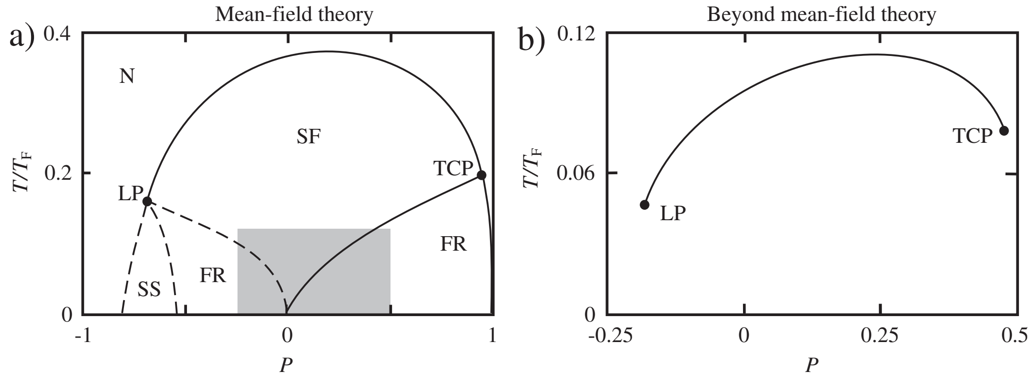

FIG. 1. Universal phase diagram for the homogeneous ^{6}Li-^{40}K mixture in the unitarity limit as a function of temperature T and polarization P. The temperature is scaled with the reduced Fermi temperature $k_B T_F = \epsilon_F = \hbar^2(3\pi^2 n)^{2/3}/2m$, where m is twice the reduced mass and n is the total particle density. The result of mean-field theory is shown in panel (a). For a majority of light ^{6}Li atoms there is a tricritical point (TCP), at which the normal state (N), the homogeneous superfluid state (SF), and the forbidden region (FR) meet each other. For a majority of heavy ^{40}K atoms there is a Lifshitz point (LP), where there is an instability towards supersolidity (SS). The size of the supersolid stability region is not calculated within our theory and the dashed lines are therefore only guides to the eye. The grey area sets the scale for panel (b), where fluctuation effects are taken into account to calculate the location of the Lifshitz and the tricritical point more accurately.

only finds a tricritical point, in agreement with experiments [6].

In first instance, all these expectations follow from mean-field theory, which is useful for a qualitative description of the physics. However, it cannot be trusted quantitatively in the unitary regime, since it vastly overestimates critical temperatures in that case. It is thus important to understand how much these are lowered by fluctuation effects. In the mass-balanced case two effects are dominant, namely, the fermionic self-energies and the screening of the interaction due to particle-hole fluctuations [17]. Taking these into account gives in an intuitive manner results that compare well with Monte Carlo calculations [18] and experiment [6]. We find that an extension of this procedure to the ^{6}Li-^{40}K mixture leads to a reduction of the mean-field critical temperatures by an experimentally relevant factor of 3. This makes it more difficult, but not impossible, to reach the superfluid regime. Moreover, the presence of the Lifshitz point in the phase diagram is unaffected by the fluctuations, allowing for an experimental study of supersolidity in the ^{6}Li-^{40}K mixture.

Phase diagram.—The critical properties of the superfluid transition in a fermionic mixture are determined by the effective Landau theory for the superfluid order parameter $\Delta(\mathbf{x})$. Although we consider no external potential, the order parameter may still vary in space due to a spontaneous breaking of translational symmetry. Close to the continuous superfluid transition, we expand the exact effective thermodynamic potential as

$$\Omega[\Delta] = \int d\mathbf{x}\left\{\gamma|\nabla\Delta|^2 + \alpha|\Delta|^2 + \frac{\beta}{2}|\Delta|^4 + \ldots\right\}, \quad (1)$$

where the challenge is to express the expansion parameters in terms of the temperature T and the atomic chemical potentials $\mu_\pm$. The upper (lower) sign refers to the light ^{6}Li (heavy ^{40}K) atoms. A phase transition has occurred when the global minimum of Ω is located at a nonzero order parameter $\langle\Delta(\mathbf{x})\rangle$, which describes a condensate of pairs. When $\gamma(T)$ is positive, the pairs have a positive effective mass and their center-of-mass state of lowest energy is at zero momentum. Then, we can consider a homogeneous pairing field Δ, for which a second-order transition occurs at a critical temperature T_c determined by $\alpha(T_c) = 0$.

A continuous transition only occurs when the minimum at small values of $\langle\Delta\rangle$ is global, which is not necessarily the case. The expansion of Ω may contain higher powers of $|\Delta|^2$ that have negative coefficients, leading to a first-order transition with a jump in the order parameter when $\Omega[0] = \Omega[\langle\Delta\rangle]$. Second-order behavior turns into first-order behavior when $\beta(T)$ becomes negative, so that the temperature T_{c3} at the tricritical point (TCP) is determined by $\alpha(T_{c3}) = 0$ and $\beta(T_{c3}) = 0$. Another intriguing possibility is that not $\beta(T)$, but rather $\gamma(T)$ goes to zero. This leads to a Lifshitz point (LP), which is thus determined by $\alpha(T_L) = 0$ and $\gamma(T_L) = 0$. Since the effective mass of the Cooper pairs becomes negative below the Lifshitz point, it is energetically favorable for them to have kinetic energy and form a superfluid at nonzero momentum. This can be established in many ways, namely, through a standing wave [14] or a more complicated superposition of plane waves [19,20]. Because of the variety of possibilities it is hard to predict which lattice structure is most favorable. However, the fact that they all emerge from the Lifhitz point facilitates the experimental search for supersolidity in the ^{6}Li-^{40}K mixture. Moreover, a nonzero gap $\langle\Delta\rangle$ gives rise to a sizeable superfluid fraction, showing that the LO-like incommensurate supersolid is very different from the commensurate supersolid studied in ^{4}He.

We continue our discussion at the mean-field level, which is useful for further explaining the relevant physics. The starting point is the BCS thermodynamic potential density for the ^{6}Li-^{40}K mixture with masses $m_\pm$ [13],

$$\omega_{\mathrm{BCS}}[\Delta;\mu_\sigma] = \int \frac{d\mathbf{k}}{(2\pi)^3}\left\{\epsilon(\mathbf{k}) - \mu - \hbar\omega(\mathbf{k}) + \frac{|\Delta|^2}{2\epsilon(\mathbf{k})} - k_B T \sum_{\sigma=\pm} \ln(1 + e^{-\hbar\omega_\sigma(\mathbf{k})/k_B T})\right\}, \quad (2)$$

where we introduced the average chemical potential $\mu = (\mu_+ + \mu_-)/2$, the difference $h = (\mu_+ - \mu_-)/2$, and the reduced kinetic energy $\epsilon(\mathbf{k}) = \hbar^2\mathbf{k}^2/2m$ with $m = 2m_+m_-/(m_+ + m_-)$. The Bogoliubov quasiparticle dispersions become $\hbar\omega_\sigma(\mathbf{k}) = \hbar\omega(\mathbf{k}) - \sigma[2h - \epsilon_+(\mathbf{k}) + \epsilon_-(\mathbf{k})]/2$ with $\hbar\omega(\mathbf{k}) = \sqrt{[\epsilon(\mathbf{k}) - \mu]^2 + |\Delta|^2}$ and $\epsilon_\sigma(\mathbf{k}) = \hbar^2\mathbf{k}^2/2m_\sigma$. We can now apply the exact critical conditions to ω_{BCS} and obtain the mean-field phase diagram. Although the BCS potential neglects fluctuations in the order parameter, it is expected that fluctuation effects only result in quantitative corrections. This expectation stems from the strongly interacting experiments for the mass-balanced case, for which the mean-field diagram is topologically correct [6]. The coefficients determining the second-order phase transition and the tricritical point are readily calculated as $\alpha = \partial\omega_{\mathrm{BCS}}[0;\mu_\sigma]/\partial|\Delta|^2$ and $\beta = \partial^2\omega_{\mathrm{BCS}}[0;\mu_\sigma]/\partial^2|\Delta|^2$. The results are shown in the phase diagram of Fig. 1(a). The polarization is defined as $P = (n_+ - n_-)/(n_+ + n_-)$, while the particle densities are determined by $n_\sigma = -\partial\omega_{\mathrm{BCS}}[\langle\Delta\rangle;\mu_\sigma]/\partial\mu_\sigma$. Therefore, the polarization is discontinuous simultaneously with the order parameter, which gives rise to a forbidden region (FR) below the tricritical point.

From Fig. 1(a), we see that the mean-field phase diagram also contains a Lifshitz point. It is calculated from the noninteracting Green's function for the Cooper pairs $G_\Delta(\mathbf{k}, i\omega_n)$. In the normal state, this propagator is given by $\hbar G_\Delta^{-1}(\mathbf{k}, i\omega_n) = 1/T^{2B} - \hbar\Xi(\mathbf{k}, i\omega_n)$, where $T^{2B} = 4\pi a\hbar^2/m$ with a the diverging scattering length, while Ξ is the so-called ladder diagram, given by

$$\hbar\Xi(\mathbf{k}, i\omega_n) = \int \frac{d\mathbf{k}'}{(2\pi)^3}\left\{\frac{1}{2\epsilon(\mathbf{k}')} + \frac{1 - N_+(\mathbf{k}') - N_-(\mathbf{k} - \mathbf{k}')}{i\hbar\omega_n - \epsilon_+(\mathbf{k}') - \epsilon_-(\mathbf{k} - \mathbf{k}') + 2\mu}\right\} \quad (3)$$

with $N_\sigma(\mathbf{k}) = 1/[e^{(\epsilon_\sigma(\mathbf{k}) - \mu_\sigma)/k_B T} + 1]$ the Fermi distributions. Note that the mean-field expression for α is equal to $-\hbar G_\Delta^{-1}(\mathbf{0}, 0)$, while we have that $\gamma = -\partial\hbar G_\Delta^{-1}(\mathbf{0}, 0)/\partial\mathbf{k}^2 = 0$ at the Lifshitz point. What precisely happens below the Lifshitz point is an intriguing question for further research. In Fig. 1(a), we have sketched a simple scenario, where there is a second-order transition from the normal to the supersolid phase, for which the condition is $G_\Delta^{-1}(\mathbf{k}_{\mathrm{SS}}, 0) = 0$ with $\mathbf{k}_{\mathrm{SS}}$ the wave vector of the supersolid. However, this transition can in principle be of first order, where the realized supersolid periodicity can also contain more than one wave vector [19]. Moreover, the transition from supersolidity to the homogeneous superfluid phase is also expected to be of first order. The calculation for the stability regions of all possible supersolid lattices is beyond the scope of this Letter, such that the dashed lines in Fig. 1(a) are merely guides to the eye.

Strong interactions.—Having established that within mean-field theory a tricritical point dominates the phase diagram when there is an abundance of light ^{6}Li atoms, while a Lifshitz points is present when there is an abundance of heavy ^{6}K atoms, the question arises whether this interesting physics remains when we take fluctuation effects into account. Answering this question also leads to more quantitative predictions for future experiments. The normal equation of state at unitarity is known to be strongly affected by fluctuations [21]. Since this equation of state exactly follows from the fermionic self-energies, we first try to take these accurately into account. We achieve this through a simple construction that gives excellent agreement with Monte Carlo results, and for which we only need to know the self-energy $\hbar\Sigma_\sigma$ of a single σ atom in a sea of $-\sigma$ atoms. At zero temperature, it is given by $\hbar\Sigma_\sigma = -c_\sigma\mu_{-\sigma}$. The coefficients can be calculated within the ladder approximation [22] giving $c_+ = 2.2$ and $c_- = 0.44$, or with a renormalization-group approach [17] giving $c_+ = 2.0$ and $c_- = 0.34$, while Monte Carlo calculations lead to $c_+ = 2.3$ and $c_- = 0.36$ [23]. Noting that these approaches agree rather well, we use the Monte Carlo

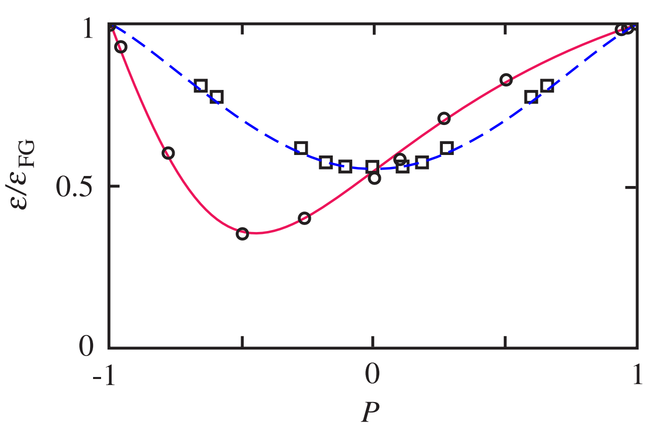

FIG. 2 (color online). Equations of state for the zero-temperature normal state of the ^{6}Li-^{40}K mixture (full line) and the mass-balanced mixture (dashed line) in the unitarity limit. The Monte Carlo results for the ^{6}Li-^{40}K mixture by Gezerlis *et al.* [23] are shown by circles, while the Monte Carlo results for the mass-balanced mixture by Lobo *et al.* [25] are shown by squares. The energy density ϵ is scaled with the ideal gas result $\epsilon_{\mathrm{FG}} = 3(\epsilon_{F+}n_+ + \epsilon_{F-}n_-)/5$ with $\epsilon_{F\sigma} = \hbar^2(6\pi^2 n_\sigma)^{2/3}/2m_\sigma$. The deviations from one thus show the strong interaction effects.

results for the rest of the calculation, since they effectively incorporate all Feynman diagrams. Moreover, $\hbar\Sigma_{-\sigma} = 0$ because the majority atoms are unaffected by the single minority atom. The chemical potential of the minority particle is then given by $\mu_\sigma = \hbar\Sigma_\sigma$.

Next, we define renormalized chemical potentials as $\mu'_\sigma = \mu_\sigma + c_\sigma \mu'^2_{-\sigma}/(\mu'_\sigma + \mu'_{-\sigma})$ [8]. Two important solutions to these equations are such that the chemical potential of one species $(-\sigma)$ is not renormalized, $\mu'_{-\sigma} = \mu_{-\sigma}$, while the renormalized chemical potential of the other species is zero, i.e., $\mu'_\sigma = \mu_\sigma + c_\sigma \mu_{-\sigma} = 0$. These two solutions correspond precisely to the two extremely imbalanced limits. By using the renormalized chemical potentials in the mean-field thermodynamic potential, we can calculate the full normal equation of state by using the equation for the densities $n_\sigma = -\partial\omega_{\rm BCS}[0; \mu'_\sigma]/\partial\mu_\sigma$. The comparison with the Monte Carlo equation of state is shown in Fig. 2 and the agreement is excellent. We also show the comparison for the mass-balanced case, where both ladder and Monte Carlo calculations give $c_\pm = 0.61$. The agreement shows that our construction captures the full thermodynamics of the strongly interacting normal state without any free parameters. Since we do not expect the coefficients $c_\pm$ to depend strongly on temperature, we can also use our method at low temperatures. Moreover, it is easily extended to other mass ratios and to the superfluid state [8].

The above discussion shows that we effectively account for all fluctuations in the normal state. However, there is a second effect of particle-hole fluctuations which affects the superfluid state. Namely, the change in the coefficient α due to screening of the interspecies interaction [24]. We account for this screening by replacing the two-body transition matrix T^{2B} with an effective transition matrix that includes the so-called bubble sum. We thus have that $1/T^{\rm eff} = 1/T^{2B} - \hbar\Pi(\mathbf{0}, 0)$, where

$$\hbar\Pi(\mathbf{0}, 0) = \int \frac{d\mathbf{k}'}{(2\pi)^3} \frac{N_+(\mathbf{k}') - N_-(\mathbf{k}')}{2h' - \epsilon_+(\mathbf{k}') + \epsilon_-(\mathbf{k}')}. \quad (4)$$

Since now $\alpha = -\hbar G_\Delta^{-1}(\mathbf{0}, 0) = -1/T^{\rm eff} + \hbar\Xi(\mathbf{0}, 0)$, the equation for the critical temperature, $\alpha = 0$, becomes $-\hbar\Xi(\mathbf{0}, 0) = \hbar\Pi(\mathbf{0}, 0)$, where we use renormalized chemical potentials to include the self-energy effects. If we apply this procedure to the mass and population-balanced case we find $T_c = 0.18 T_F$ and $\mu(T_c) = 0.52\epsilon_F$, which is to be compared with the Monte Carlo results $T_c = 0.15 T_F$ and $\mu(T_c) = 0.49\epsilon_F$ [18]. Moreover, we find for the mass-balanced tricritical point that $k_B T_{c3} = 0.09\epsilon_{F+}$ and $P_{c3} = 0.25$, which agrees with the experimental data [6]. Returning to the ^{6}Li-^{40}K mixture and using the same conditions for the tricritical point and the Lifshitz point as before, we find the result in Fig. 1(b). Note that the critical temperatures are lowered by about a factor of 3 due to the screening and the self-energy effects. Also the locations of the Lifshitz point and the tricritical point have drastically changed, since now we find $T_{c3} = 0.08 T_F$ and $P_{c3} = 0.47$, while $T_L = 0.05 T_F$ and $P_L = -0.18$.

Conclusion.—We have considered the experimentally available ^{6}Li-^{40}K mixture at unitarity, where we incorporated self-energy effects to reproduce at zero temperature the normal equation of state from Monte Carlo calculations. By also including the effect of screening on the critical temperature, we have made quantitative predictions for the phase diagram, which contains both a Lifshitz and a tricritical point. At weaker attractions the Lifshitz point remains present, although its temperature gets exponentially suppressed. Below it, various supersolid phases are competitive [19,20] and a rich phase structure is expected. We hope that this Letter will stimulate new experimental research on supersolidity.

We thank Jeroen Diederix for stimulating discussions and Alex Gezerlis for kindly providing us with their Monte Carlo data. This work is supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM) and the Nederlandse Organisatie voor Wetenschaplijk Onderzoek (NWO).

*K.B.Gubbels@uu.nl

[1] M. Greiner *et al.*, Nature (London) **426**, 537 (2003).
[2] S. Jochim *et al.*, Science **302**, 2101 (2003).
[3] C. A. Regal *et al.*, Phys. Rev. Lett. **92**, 040403 (2004).
[4] M. W. Zwierlein *et al.*, Science **311**, 492 (2006).
[5] G. B. Partridge *et al.*, Science **311**, 503 (2006).
[6] Y. Shin *et al.*, Nature (London) **451**, 689 (2008).
[7] K. B. Gubbels *et al.*, Phys. Rev. Lett. **97**, 210402 (2006).
[8] J. M. Diederix *et al.*, arXiv:0907.0127.
[9] E. Wille *et al.*, Phys. Rev. Lett. **100**, 053201 (2008).
[10] A.-C. Voigt *et al.*, Phys. Rev. Lett. **102**, 020405 (2009).
[11] K.-K. Ni *et al.*, Science **322**, 231 (2008).
[12] K. Góral *et al.*, Phys. Rev. Lett. **88**, 170406 (2002).
[13] M. M. Parish *et al.*, Phys. Rev. Lett. **98**, 160402 (2007).
[14] A. I. Larkin and Y. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **47**, 1136 (1964).
[15] P. Fulde and R. A. Ferrell, Phys. Rev. **135**, A550 (1964).
[16] A. Bulgac and M. M. N. Forbes, Phys. Rev. Lett. **101**, 215301 (2008).
[17] K. B. Gubbels and H. T. C. Stoof, Phys. Rev. Lett. **100**, 140407 (2008).
[18] E. Burovski *et al.*, Phys. Rev. Lett. **96**, 160402 (2006).
[19] C. Mora and R. Combescot, Phys. Rev. B **71**, 214504 (2005).
[20] N. Yoshida and S.-K. Yip, Phys. Rev. A **75**, 063601 (2007).
[21] C. A. R. Sá de Melo *et al.*, Phys. Rev. Lett. **71**, 3202 (1993).
[22] R. Combescot *et al.*, Phys. Rev. Lett. **98**, 180402 (2007).
[23] A. Gezerlis *et al.*, Phys. Rev. Lett. **103**, 060403 (2009).
[24] L. P. Gor'kov and T. K. Melik-Barkhudarov, Sov. Phys. JETP **13**, 1018 (1961).
[25] C. Lobo *et al.*, Phys. Rev. Lett. **97**, 200403 (2006).