Validity of the Gor'kov expansion near the upper critical field in type II superconductors

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Abstract.   We have examined the validity of the Gor'kov expansion in the strength of the order parameter of type II superconductors near the upper critical field. Although the degeneracy of the electron levels in a magnetic field gives non-perturbative terms in the solution to the Bogoliubov–de Gennes equations we find, contrary to recent claims, that these non-perturbative terms cancel in the expression for the thermodynamic potential, and that the traditional Gor'kov theory is correct sufficiently close to H_{c2} at finite temperature. We have derived conditions for the validity of the Gor'kov theory which essentially state that the change in the quasiparticle energies as compared to the normal-state energies cannot be too large compared to the temperature.

1. Introduction

Recently the view has been advocated that the Gor'kov expansion describing type II superconductors close to the upper critical field H_{c2} may be invalid [1]. Even within the mean-field approximation there is a possibility of non-perturbative effects arising from the degeneracy of the Landau levels for electrons moving in a magnetic field. This degeneracy means that even a small perturbation (e.g. superconducting order) can change the quasiparticle levels significantly as compared to the normal state. This effect has been proposed as a mechanism for the breakdown of the standard perturbation theory describing type II superconductors even close to H_{c2}. This non-perturbative effect should give rise to effects such as tails of residual superconductivity above the usual H_{c2}, the possibility of the superconducting transition being first order, and unusual behaviour of the heat capacity, magnetization, etc close to the phase boundary [1]. In this work we have examined this possibility. We show that for $T = 0$ there are indeed terms not contained in the Gor'kov expansion for the difference between the ground-state energy of the mixed state and the normal state. This is in agreement with the results obtained by Bahcall [1] and is no surprise since the Gor'kov expansion is essentially a high-temperature series. However, for $T \neq 0$ we show that the non-perturbative terms in the difference $\Omega_S - \Omega_N$ between the thermodynamic potentials in the mixed state and the normal state vanish, and indeed that the Gor'kov expansion is a convergent series for the superconducting order $\Delta(r)$ not too large. We thus prove incorrect the claim of Bahcall that there is a non-perturbative third-order term in the expression for $\Omega_S - \Omega_N$. We have derived some criteria for the convergence radius of the Gor'kov expansion in the order parameter. A comparison between the results of the Gor'kov expansion and a numerical solution of the corresponding Bogoliubov–de Gennes (BdG) equations [2] confirms our conclusions. In this paper we work in two dimensions. We do not consider any fluctuation effects relevant to high-T_c superconductors [3].

2. Mean-field theory

Within the mean-field approximation the mixed state of a type II superconductor is described by the solutions to the BdG equations. In a constant magnetic field the order parameter forms an Abrikosov vortex lattice, and it is convenient to use a set of single-particle states $\phi_{N,k}$ characterized by the Landau level index N and a wavevector k in the Brillouin zone of the vortex lattice. In this basis the BdG equations split up into a set of $2N \times 2N$ secular matrix equations, one for each k, where N is the number of Landau levels participating in the pairing. In this basis the BdG equations are [4]

$$(\xi_N - E_k^\eta)u_{Nk}^\eta + \sum_M F_{kNM}v_{Mk}^\eta = 0$$
$$(-\xi_N - E_k^\eta)v_{Nk}^\eta + \sum_M F_{kMN}^* u_{Mk}^\eta = 0 \tag{1}$$

where u_{Nk}^η is the coefficient of ϕ_{Nk} for the Bogoliubov function $u_k^\eta(r)$, and v_{Nk}^η is the coefficient of $\phi_{N,-k}^*$ for the function $v_k^\eta(r)$, and $\xi_N = (N + 1/2)\hbar\omega_c - \mu$. μ is the chemical potential. The off-diagonal elements F_{kNM} are

$$F_{kNM} = \int d r \ \Delta(r)\phi(r)_{N,k}^*\phi(r)_{M,-k}^* \tag{2}$$

and the order parameter is determined self-consistently as

$$\Delta(r) = g \sum_{k\eta} u_k^\eta(r)v_k^\eta(r)^*(1 - 2f_k^\eta) \tag{3}$$

where g is the coupling strength and $f_k^\eta = (1 + \exp(E_k^\eta/k_BT))$ is the Fermi function. We neglect any finite Zeeman splitting for simplicity. Due to the translational symmetry the order parameter $\Delta(r)$ is completely characterized by a finite set of parameters Δ_j [4]. For notational simplicity we work in the lowest-Landau-level approximation (LLL) (i.e. $\Delta_{J\neq0} = 0$) in which the centre-of-mass motion of the Cooper pairs has the kinetic energy $\hbar\omega_c/2$ where ω_c is the cyclotron frequency. None of the conclusions in this paper are altered when this restriction is relaxed. When the chemical potential μ is at a Landau level (i.e. $n_f \equiv \mu/\hbar\omega_c - 1/2 =$ integer) we have, in the normal state, exact degeneracy between an electron state in the Landau level $n_f + m$ and a hole state in the Landau level $n_f - m$. Likewise when the chemical potential is exactly in between two Landau levels such that $n_f = n + 1/2$ there is degeneracy between an electron in a level $n_f + m + 1/2$ and a hole in a level $n_f - m - 1/2$. When this is the case we expect the possible non-perturbative effects of a finite order parameter to be strongest. We will show that the convergence radius for the Gor'kov equations is indeed smallest when n_f is an integer. To examine the validity of the Gor'kov expansion it is convenient to use the following expression [5] for the difference $\Omega_S - \Omega_N$ between the thermodynamic potentials of the mixed state and the normal state:

$$\Omega_S - \Omega_N = \frac{1}{g} \int d r \ |\Delta(r)|^2 - 2k_BT \sum_{Nk} \ln(\cosh(\beta E_{Nk}/2))$$
$$+ 2k_BTD \sum_N \ln(\cosh(\beta\xi_i/2)). \tag{4}$$

Here $D = VeB/(2\pi\hbar c)$ is the number of k-vectors in the Brillouin zone, V is the volume, B is the magnetic field, and $\beta = 1/k_BT$.

3. Zero temperature

To illustrate the origin of the non-perturbative effect for $T = 0$ it is sufficient to examine the case where only one Landau level participates in the pairing and n_f is an integer. In this case the positive-energy solution to equation (1) is $E_{n_f k} = |F_{kn_f n_f}|$. Equation (4) reduces to

$$E_{gS} - E_{gN} = \frac{1}{g} \int d\mathbf{r} \ |\Delta(\mathbf{r})|^2 - \sum_k E_{n_f k}. \tag{5}$$

Since $|F_{kn_f n_f}| \propto \Delta_0 \propto |\Delta(\mathbf{r})|$ we see that we obtain a linear term in $|\Delta(\mathbf{r})|$ in equation (4). This is a non-perturbative term since the Gor'kov expansion only contains even powers of the order parameter. This $T = 0$ result is unaltered when we have many Landau levels participating in the pairing, and it agrees with the result obtained by Bahcall [1]. It is a trivial consequence of the fact that we have to take the $T \to 0$ limit $k_B T \ln(2 \cosh(\beta E_{Nk}/2)) \to E_{Nk}/2$ before we perturbatively expand the result in the size of the order parameter.

4. Finite temperature

4.1. The quantum limit

For finite temperature the situation is different. It is now possible to expand $\ln(2 \cosh(\beta E_{Nk}/2))$ in powers of the order parameter and then check whether we obtain any non-perturbative terms, as proposed by Bahcall [1]. For notational simplicity we will again do the calculation in the quantum limit where only one Landau level participates in the pairing. In section 4.2 we will treat the slight modifications to our result when more than one Landau level is within the pairing width. The quasiparticle energy is now $E_{nk} = \sqrt{\xi_n^2 + |F_{knn}|^2}$. We need to expand $\ln(\cosh(\beta E_{nk}/2))$ in $|F_{knn}|^2$. Writing $\beta E_{nk}/2 = \sqrt{\epsilon^2 + z^2}$ where $\epsilon \equiv \beta \xi_n/2$ and $z = \beta |F_{knn}|/2$, we are led to consider the analytic properties of the function $\ln(\cosh(\sqrt{\epsilon^2 + z^2}))$. The poles and branch cuts in the complex plane $z \in \mathcal{C}$ determine the convergence radius r_0 for a power series in z. A simple analysis gives $r_0 = \sqrt{\epsilon^2 + \pi^2/4}$. The requirement for the convergence of a perturbation series for $\ln(2 \cosh(\beta E_{Nk}/2))$ is then

$$|F_{knn}| \leqslant \sqrt{\xi_n^2 + \pi^2 (k_B T)^2}. \tag{6}$$

This requirement is most restrictive when the Landau level is at the chemical potential ($\xi_n = 0$). We then have

$$E_k \leqslant k_B T \pi. \tag{7}$$

Furthermore, we see that only even powers of $|F_{knn}|$ will appear in the series. This is true for general μ (i.e. also when $\xi_n = 0$). So we have ruled out any non-perturbative cubic term in the expression for $\Omega_S - \Omega_N$, thereby disproving earlier predictions based on a numerical analysis [1]. Doing the expansion and comparing with a standard expression for the thermodynamic potential based on Gor'kov's equations [6] we find (not surprisingly) that it reproduces the Gor'kov series term by term. The convergence of the Gor'kov expansion is determined by equation (6). It is now clear that the Gor'kov expansion is a high-temperature series. So the breakdown of the theory for $T = 0$ is no surprise. For finite T we expect the Gor'kov series to first become unreliable when there is a Landau level at the chemical potential. This is because the requirement in equation (6) is most restrictive

when $\xi_n = 0$, and because the superconductivity and thereby the change in the quasiparticle energies (obtained by a self-consistent solution of equation (1)) is enhanced when there is a Landau level at the chemical potential [6].
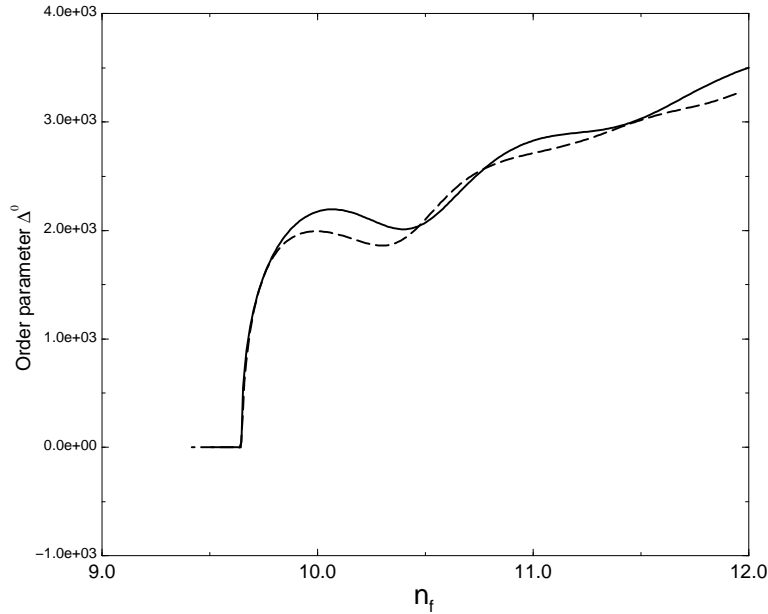

Figure 1. The order parameter Δ_0 versus $n_f = \mu/\hbar\omega_c - 1/2$ calculated numerically (solid line) and perturbatively to fourth order in Δ_0 (dotted line) for $\omega_d/\omega_c = 5$, $g/\hbar\omega_c l^2 = 8.2$ and $k_B T/\hbar\omega_c = 0.3$ when $n_f = 12$.

4.2. Several Landau levels

The above conclusions are essentially unaltered when there is more than one Landau level participating in the pairing. We calculate the quasiparticle energies from equation (1) perturbatively in F_{knm} using degenerate and non-degenerate perturbation theory. Then we expand $\ln(2\cosh(\beta E_{Nk}/2))$ in powers of the order parameter. The convergence radius for the series is again smallest when the chemical potential is at a Landau level. The only complication is that we obtain both even and odd powers of F_{knm} in the expression for the quasiparticle energies. But the odd terms cancel in the expression for $\Omega_S - \Omega_N$ due to the fact that there are two quasiparticle levels when $\xi_n \neq 0$ for which the odd powers in the expression for the energy have opposite signs. There is only one positive-energy solution for the case where $\xi_{n_f} = 0$ though. However, the odd terms from this solution vanish in the expression for $\Omega_S - \Omega_N$ due to the fact that $\partial_x^{2l+1} \ln(\cosh(x))|_{x=0} = 0$ where l is an integer. A long tedious calculation shows that we recover the standard terms in the Gor'kov series. A sufficient condition for the convergence of the Gor'kov series is

$$E_{nk} - \xi_n \leqslant \min\left[2k_B T\pi, k_B T\sqrt{\beta^2\xi_n^2 + \pi^2}\right] \tag{8}$$

which has to hold for each quasiparticle level within the pairing region. So we expect that the Gor'kov theory breaks down when significant portions of the quasiparticle bands lie
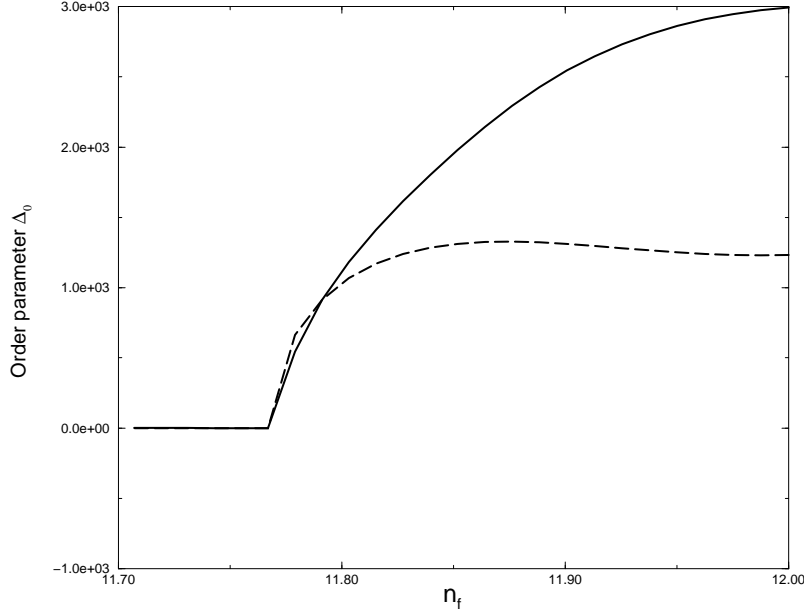
Figure 2. The order parameter Δ_0 versus $n_f = \mu/\hbar\omega_c - 1/2$ calculated numerically (solid line) and perturbatively to fourth order in Δ_0 (dotted line) for $\omega_d/\omega_c = 5$, $g/\hbar\omega_c l^2 = 7.0$ and $k_B T/\hbar\omega_c = 0.05$ when $n_f = 12$.

outside the regions defined in equation (8). It should be noted that one cannot ignore the contribution from higher quasiparticle levels to $\Omega_S - \Omega_N$ ($\xi_n \neq 0$). This is easily seen from equation (4) since

$$\ln(\cosh(\beta(\xi + \delta E)/2)) - \ln(\cosh(\beta\xi/2)) > \ln(\cosh(\beta(\delta E)/2)) \qquad \xi, \delta E > 0. \tag{9}$$

So any treatment which focuses only on the quasiparticle level at the chemical potential will ignore important contributions to Ω_s. Equation (8) can be transformed into the requirement

$$\langle |\Delta(r)|^2 \rangle \equiv \frac{1}{V} \int \mathrm{d}r \; |\Delta(r)|^2 \leqslant 2\sqrt{\pi n_f}\pi^2(k_B T)^2. \tag{10}$$

Since the Ginzburg–Landau equations are derived from the microscopical BCS theory using the Gor'kov expansion [7], it would be of interest to restate the above criterion in terms of Ginzburg–Landau parameters. Doing this we obtain

$$\frac{H_{c2} - H}{H_c(0)} \leqslant \sqrt{n_f}\pi^{1/2}(7\zeta(3))^{1/2}\beta_A \mathrm{e}^\gamma \left(\kappa - \frac{1}{2\kappa}\right)\left(\frac{T}{T_c}\right)^2. \tag{11}$$

Here $\zeta(x)$ is Riemann's zeta function, κ is the Ginzburg–Landau parameter, β_A is the Abrikosov parameter, and γ is Euler's constant. This restriction is always fulfilled for type II superconductors within the normal range of validity of the Ginzburg–Landau equations (i.e $|T - T_c|/T_c \ll 1$).

As an example of the breakdown of the perturbation series we have plotted the order parameter Δ_0 as a function of $n_f = \mu/\hbar\omega_c - 1/2$. In figure 1 we have plotted both a numerical exact solution of the BdG equations and the fourth-order perturbative result obtained using a method developed earlier [6]. We have chosen the parameters such that $\omega_d/\omega_c = 5$, $g/\hbar\omega_c l^2 = 8.2$ and $k_B T/\hbar\omega_c = 0.3$ when $n_f = 12$. As can be seen the
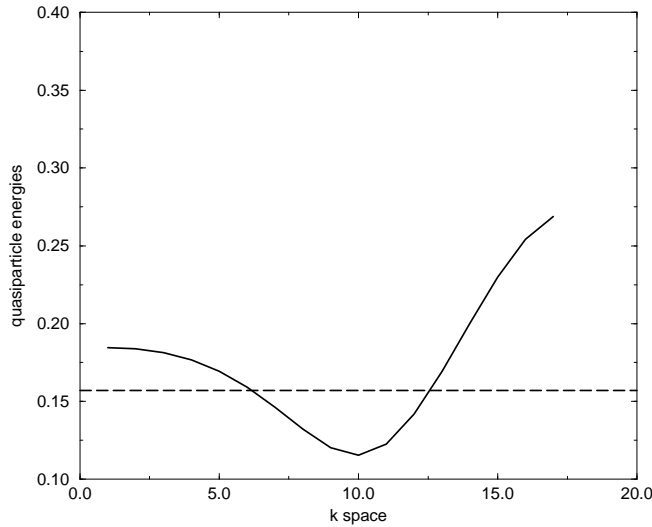
Figure 3. The lowest quasiparticle band in units of $\hbar\omega_c$ along a high-symmetry line in k-space for $n_f = 12$. The dashed line marks the boundary defined by equation (8).

perturbation theory agrees fairly well with the exact solution. The perturbative result tends to differ the most from the exact solution when the chemical potential is at a Landau level ($n_f = $ integer). This is in agreement with the above remarks. To illustrate the temperature dependence of the convergence radius of the Gor'kov series we have in figure 2 again plotted Δ_0 as a function of n_f for a very low temperature. As can be seen, the perturbation series breaks down much earlier: $\Delta_0 \simeq 1500$ for this low temperature in agreement with equation (8). In figure 3 we have plotted the lowest quasiparticle level along a high-symmetry direction in k-space when $n_f = 12$ for the parameters used in figure 2. The horizontal line gives the boundaries for $E_k - \xi$ calculated from equation (8). There are large parts of the quasiparticle band in k-space lying outside the region of convergence of the perturbation expansion, thereby explaining the observed discrepancies between perturbation theory and the exact numerical result.

5. Conclusion

In conclusion we have examined the recently debated validity of the Gor'kov expansion. The conclusion is that although the degeneracy of the normal-state levels gives large effects on the quasiparticle wavefunctions even for weak superconducting order, these effects cancel in the expression for the thermodynamic potential, and the Gor'kov expansion is correct for finite temperature. We have therefore ruled out the possibility of a non-perturbative third-order term in the expression for the thermodynamic potential. The range of validity of the Gor'kov expansion is given by equation (8), which shows that it is essentially a high-temperature expansion. This requirement is always fulfilled within the range of validity of the Ginzburg–Landau equations, leading to there being no inconsistencies. Furthermore, we have the usual requirement $|E_{nk} - \xi_n| \ll \hbar\omega_c$ for perturbation theory to work. We expect the Gor'kov expansion the break down first when the chemical potential is at a Landau level. Our results are confirmed by a comparison between the results of an exact numerical solution to the BdG equations and a Gor'kov series to fourth order in the order parameter.

Acknowledgments

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