Surface boundary conditions for the Ginzburg-Landau theory of *d*-wave superconductors

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We calculate de Gennes' extrapolation length for a *d*-wave superconductor near a surface within Fermi-liquid theory. The extrapolation length depends critically on the orientation of the surface relative to the crystal axes and on the surface roughness. This sensitivity of the boundary conditions for a *d*-wave order parameter to surface conditions is not found in traditional *s*-wave superconductors, and is a signature of anisotropic pairing with a changing sign of the order parameter along the Fermi surface. de Gennes' method is used to calculate the reduction of T_c in thin strips of high-T_c superconductors.

I. INTRODUCTION

The Ginzburg-Landau (GL) theory is among the most successful and versatile theories of superconductivity. It has amazing predictive power which led, for example, to the discovery of the vortex state by Abrikosov[1] and of the phenomenon of surface superconductivity by Saint-James and de Gennes.[2] In addition, it is the only theory which is simple enough to handle very complex superconducting phenomena such as the response of unconventional superconductors to a magnetic field.[3,4] In view of the ongoing controversy as to the proper microscopic approach to high-T_c superconductivity, it should be emphasized that a fundamental phenomenological theory such as the GL theory holds for any of the commonly discussed microscopic mechanisms. A microscopic theory of high-T_c superconductivity enables us to calculate the phenomenological parameters of the GL theory (such as the symmetry of the order parameter, the critical temperature, the coherence length, etc.) but will leave the general form of the GL theory unchanged.

We are interested here in the GL theory for layered *d*-wave superconductors, and its potential application to the high-T_c cuprates. The *d*-wave model of superconductivity is in fairly good agreement with most of the experimental data on high-T_c superconductors,[5] and thus competes with various alternative models[6–10] for the proper microscopic approach to high-T_c superconductivity. In contrast to the microscopic models, which are controversial and disputed, the good accuracy and reliability of the phenomenological GL model is undisputed. The minimum energy solution of the GL equation is a good approximation to the order parameter in thermodynamic equilibrium provided fluctuations can be neglected. Fluctuations are included in the GL theory if the GL free energy is used as the free energy functional in the Ginzburg-Landau-Wilson functional integrals. Near T_c this theory is considered an exact theory of the thermodynamics of superconductors. Being restricted to the temperature range near T_c and to thermodynamic phenomena is not the only disadvantage of the GL theory. In view of the controversy on the symmetry of the superconducting state in high-T_c materials another disadvantage of the GL model should be mentioned. Many phenomena which are accessible to GL theories do not distinguish superconductors with different symmetries. All types of pairing which are presently discussed in the context of high-T_c materials lead to a one-component order parameter with the same bulk GL equations. As a consequence, bulk experiments on thermodynamic properties near T_c (heat capacity, phase diagrams, vortex structures, vortex lattice, etc.) do not carry information on the symmetry of the GL order parameter. This is different from the GL theories of heavy fermion superconductors which could, for example, explain the anomalous phase diagram near T_c.[11] The GL boundary conditions at surfaces and interfaces are more selective. They depend, in general, on the symmetry of the order parameter. The most prominent examples are the Josephson coupling energy in *d*-wave superconductors with tetragonal crystal symmetry,[12,13] anomalies in the tunneling spectra,[14–16] and spontaneous breaking of time-reversal symmetry.[17] The Josephson couplings between a $d_{x^2-y^2}$ superconductor (B_1 symmetry) and an *s*-wave superconductor (A_1 symmetry) have opposite signs at the *a* and *bx* interfaces, whereas two *s*-wave superconductors have the same coupling constants at these interfaces. The sign change is a substantial qualitative difference whose measurement in tetragonal systems would be a direct proof of an order parameter of nontrivial ($\neq A_1$) symmetry. These fundamental effects require the Josephson coupling to a different superconductor or the same but differently oriented superconductor, and will not occur at the surface of a superconductor in contact with an insulator. Nevertheless, one expects significant quantitative differences between *s*-wave and *d*-wave superconductors near such surfaces for the following reasons. Following de Gennes[18] one describes the effects of a surface on the superconducting state by an extrapolation length b. An isotropic conventional superconductor has $b=\infty$ at a nonmagnetic, fully reflecting surface. On the other hand, one expects for *d*-wave superconductors and other strongly anisotropic superconductors[15,16] a short extrapolation length of the order of the T-independent coherence length. The reason is that surface scattering is pair breaking in these systems and pulls down the order parameter in the vicinity of the surface. The actual strength of the pair breaking effect is expected to depend on the quality of the surface (specular or rough) and on its orientation with respect to the anisotropic order parameter.

We calculate in this article the extrapolation length for the

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GL model of d-wave superconductors from the Fermi-liquid theory of superconductivity. The extrapolation length can be obtained from classical correlation functions of Landau's quasiparticle excitations in the normal state.[19] In Sec. II we present the quasiclassical theory of the extrapolation length for singlet superconductors with arbitrary quasiparticle band structure, pairing symmetry, and surface quality. In Sec. III we introduce the d-wave model and our model surfaces, and derive de Gennes' kernel $\mathscr{K}$ for d-wave pairing. de Gennes' kernel describes superconductors near a second-order transition to the normal state and can be used, for example, to study the effect of impurities, surfaces, and interfaces on T_c or on the critical fields H_{c2} and H_{c3}. We study here the effects of surfaces, and calculate from de Gennes' kernel (a) the dependence of the extrapolation length on the quality and orientation of a surface and (b) the size effect on T_c, specifically its reduction in a slab. The results are summarized and discussed in Sec. IV.

II. QUASICLASSICAL APPROACH

A. General theory

We assume in the following that the conduction electrons in high-T_c cuprates can be described by the Fermi-liquid theory, and calculate the boundary conditions for the GL order parameter from the Fermi-liquid theory of anisotropic superconductors. The most powerful formulation of the Fermi-liquid theory of superconductivity is the ''quasiclassical theory,'' which may be interpreted as the generalization of Landau's transport equation for normal Fermi liquids to the superconducting state. Like Landau's transport equation, which is basically a classical equation, the quasiclassical theory has to a large degree the structure of a classical transport theory. An early version of a quasiclassical approach to superconductivity is de Gennes' method of correlation functions.[19,20] de Gennes discovered that the leading order terms in an expansion in powers of the superconducting order parameter can be calculated from correlation functions of classical particles moving with Fermi velocity. He was able to solve, with this method, a variety of problems of superconductivity near surfaces.[19] de Gennes' method was reformulated in terms of a classical Boltzmann transport equation by Lüders and Usadel.[20] They introduced the boundary conditions at surfaces and interfaces, originally designed for a Boltzmann distribution function, into the theory of superconductivity. Both de Gennes' method and the Boltzmann equation approach were restricted to equilibrium phenomena near a second-order transition to the superconducting phase. The breakthrough in the Fermi-liquid theory of superconductivity came with the publications by Eilenberger,[21] Larkin and Ovchinnikov,[22–24] and Eliashberg.[25] They showed that de Gennes' quasiclassical method can be generalized, and that the complete theory of superconductivity in Fermi liquids can be formulated in terms of quasiclassical transport equations. This theory covers the full temperature range of interest and equilibrium phenomena, as well as linear and nonlinear dynamics out of equilibrium. We use here the quasiclassical theory in the notation described in Refs. 26,27.

In order to keep contact with other papers on the quasiclassical theory of d-wave superconductivity[28,29,15,16] we will start from the full quasiclassical equations, and derive the GL equations including the boundary conditions by an expansion in $T_c - T$. The quasiclassical equations expanded to first order in both the microscopic order parameter $\Delta(\vec{p}_f,\vec{R})$ and the off-diagonal quasiclassical propagator $f^M(\vec{p}_f,\vec{R};\epsilon_n)$ have the form

$$(2\epsilon_n + \hbar \vec{v}_f \cdot \vec{\nabla}_R) f^M(\vec{p}_f,\vec{R};\epsilon_n) - 2\pi\Delta(\vec{p}_f,\vec{R}) = 0 . \quad (1)$$

We use the Matsubara technique for equilibrium phenomena. This is indicated by a superscript M on the propagator, and its dependence on the discrete Matsubara energies, $\epsilon_n = (2n+1)\pi k_B T$. Equation (1) is a first-order linear differential equation for $f^M(\vec{p}_f,\vec{R};\epsilon_n)$, with an inhomogeneity $\propto \Delta(\vec{p}_f,\vec{R})$. The spatial derivative in Eq. (1) is in the direction of the Fermi velocity $\vec{v}_f$, which is a function of the Fermi momenta $\vec{p}_f$. The variables ϵ_n and $\vec{p}_f$ may be considered as parameters of the differential equation. The transport equation (1) must be supplemented by the BCS gap equation

$$\Delta(\vec{p}_f,\vec{R}) = 2k_B T \sum_{\epsilon_n>0} \int d^2p_f' \; n(\vec{p}_f') \times V_{\mathrm{BCS}}(\vec{p}_f,\vec{p}_f') f^M(\vec{p}_f',\vec{R};\epsilon_n), \quad (2)$$

where $V_{\mathrm{BCS}}(\vec{p}_f,\vec{p}_f')$ is the dimensionless pairing interaction, and $\int d^2p_f$ denotes a normalized integral over the Fermi surfaces $[\int d^2p_f \, n(\vec{p}_f) = 1]$. The surface element d^2p_f is weighted in these integrals by the local density of states, $n(\vec{p}_f)$. The total density of states is included, as a factor, in the dimensionless interaction. The momentum dependence of the pairing interaction determines the symmetry and anisotropy of the microscopic order parameter $\Delta(\vec{p}_f,\vec{R})$.

The differential equation (1) requires, for a finite system, boundary conditions for f^M at surfaces. The general boundary condition for elastic reflection at surfaces is[20]

$$f^M(\vec{p}_f^{\,\mathrm{out}},\vec{R};\epsilon_n) = \int d^2p_f^{\,\mathrm{in}} \; n(\vec{p}_f^{\,\mathrm{in}}) R(\vec{p}_f^{\,\mathrm{out}},\vec{p}_f^{\,\mathrm{in}}) f^M(\vec{p}_f^{\,\mathrm{in}},\vec{R};\epsilon_n), \quad (3)$$

where $R(\vec{p}_f^{\,\mathrm{out}},\vec{p}_f^{\,\mathrm{in}})$ is the probability for a normal state quasiparticle moving towards the surface with momentum $\vec{p}_f^{\,\mathrm{in}}$ being scattered into an outgoing quasiparticle with momentum $\vec{p}_f^{\,\mathrm{out}}$. The quasiparticle current into the surface and away from it must cancel each other (conservation of the number of quasiparticles), which leads to the condition[20]

$$\int d^2p_f^{\,\mathrm{out}} \; n(\vec{p}_f^{\,\mathrm{out}}) R(\vec{p}_f^{\,\mathrm{out}},\vec{p}_f^{\,\mathrm{in}}) v_f^{\perp}(\vec{p}_f^{\,\mathrm{out}}) = -v_f^{\perp}(\vec{p}_f^{\,\mathrm{in}}). \quad (4)$$

We used the notation $v_f^{\perp}$ for the component of the Fermi velocity perpendicular to the surface. Equations (1), (2), and (3) form a closed set of equations. They always have the noninteresting, trivial solution $\Delta \equiv 0$. Nontrivial solutions will be found for certain discrete temperatures, whose largest one is the physical transition temperature. For instance, the bulk transition temperature T_c^0 is obtained by solving Eqs. (1), (2) for an infinite system. The solution Δ^0 is independent of $\vec{R}$, and one obtains the following equation for T_c^0

$$\Delta^0(\vec{p}_f)=2\pi k_B T_c^0 \sum_{\epsilon_n>0} \int d^2p_f'\; n(\vec{p}_f')V_{\rm BCS}(\vec{p}_f,\vec{p}_f')\frac{\Delta^0(\vec{p}_f')}{\epsilon_n}. \tag{5}$$

This equation pins down T_c^0 and the momentum dependence of the bulk microscopic order parameter $\Delta^0(\vec{p}_f)$. For convenience, we normalize $\Delta^0(\vec{p}_f)$ to

$$\int d^2p_f'\; n(\vec{p}_f')|\Delta^0(\vec{p}_f')|^2=1\,. \tag{6}$$

Since the anisotropy of the microscopic order parameter is pinned to the crystal lattice, the momentum dependence of $\Delta^0(\vec{p}_f,\vec{R})$ is fixed in the GL range, and one can separate the dependencies on $\vec{p}_f$ and $\vec{R}$:

$$\Delta(\vec{p}_f,\vec{R})=\Delta^0(\vec{p}_f)\times\Psi(\vec{R}). \tag{7}$$

The function $\Psi(\vec{R})$ is conveniently chosen as the GL order parameter, and one finds the following bulk GL equations:

$$\frac{T_c^0-T}{T_c^0}\Psi(\vec{R})+\left(\vec{\nabla}-i\frac{2e}{\hbar c}\vec{A}(\vec{R})\right)_\alpha \times(\xi^2)_{\alpha\beta}\left(\vec{\nabla}-i\frac{2e}{\hbar c}\vec{A}(\vec{R})\right)_\beta\Psi(\vec{R})=0\,, \tag{8}$$

where $\vec{A}$ is the vector potential, and the coherence-length tensor $(\xi^2)_{\alpha\beta}$ is given by the integral

$$(\xi^2)_{\alpha\beta}=\frac{7\zeta(3)}{4}\xi_0^2\int d^2p_f\; n(\vec{p}_f)|\Delta_0(\vec{p}_f)|^2\frac{v_{f\alpha}(\vec{p}_f)v_{f\beta}(\vec{p}_f)}{\langle v_f^2\rangle}, \tag{9}$$

where $\langle v_f^2\rangle=\int d^2p_f\; n(\vec{p}_f)|\vec{v}_f(\vec{p}_f)|^2$, and we introduced a temperature-independent coherence length ξ_0 by

$$\xi_0=\frac{\hbar\langle v_f^2\rangle^{1/2}}{2\pi k_B T_c^0}. \tag{10}$$

The result (9) follows directly from Eqs. (1), (2), (5).

Substantially more involved is the calculation of the extrapolation length. Phenomenologically one introduces[18] the extrapolation length $b(\hat{n}_{\rm surf})$ by starting from the GL surface energy[30]

$$\Omega_{\rm surf}=N_f\int dF\; a(\vec{n},\vec{R}_{\rm surf})|\Psi(\vec{R}_{\rm surf})|^2, \tag{11}$$

where we factorized out the density of states factor N_f for convenience. The integral $\int dF$ is a surface integral over the sample surface, and the length $a(\vec{n},\vec{R}_{\rm surf})$ is a phenomenological parameter which measures the strength of the pair breaking at $\vec{R}_{\rm surf}$ induced by a surface with surface normal $\vec{n}$. A parameter $a=0$ means no pair breaking, $a=\infty$ means infinitely strong pair breaking, and a negative a would mean an enhancement of superconductivity at the surface. The boundary condition for Ψ is obtained by minimizing the bulk GL energy together with the surface energy, and one obtains

$$\Psi(\vec{R}_{\rm surf})=-(\vec{n}_{\rm surf})_\alpha\frac{\xi^2_{\alpha\beta}}{a(\vec{n},\vec{R}_{\rm surf})}\nabla_\beta\Psi(\vec{R}_{\rm surf}). \tag{12}$$

The tensor $\xi^2_{\alpha\beta}/a(\vec{n},\vec{R}_{\rm surf})$ generalizes the scalar extrapolation length b to anisotropic systems. We are interested here, in particular, in the dependence of a on the orientation $(\vec{n})$ of the surface with respect to the anisotropy axes of the microscopic order parameter. This dependence can be measured, in principle, by varying the surface orientation. Such experiments would give information on the anisotropy of the microscopic order parameter, and thus provide some insight into the type of pairing in high-T_c superconductors.

B. Slab geometry

The pair breaking effect at surfaces leads to a size effect on T_c; small samples will have a reduced T_c. The reduction of T_c depends on the size and shape of the sample, and on the quality of its surfaces. For simplicity we consider here a slab of width $L\gg\xi_0$ cut from a perfect crystal. The normal to the surfaces shall have a fixed orientation (unit vector $\vec{n}$) with respect to the crystal axes. We assume homogeneity along the slab which leads to the following solution of the GL equation (8) with the boundary conditions (12):

$$\Psi(x)=\sin\left(\frac{x+b_\perp}{\xi_\perp(T)}\right), \tag{13}$$

where $\xi_\perp(T)$ is the GL coherence length perpendicular to the slab,

$$\xi_\perp(T)=\sqrt{\frac{T_c^0}{T_c^0-T_c}}\xi_\perp\,, \tag{14}$$

$b_\perp$ the corresponding extrapolation length,

$$b_\perp=\frac{\xi_\perp^2}{a(\vec{n})}, \tag{15}$$

and $\xi_\perp$ the T-independent perpendicular coherence length, $\xi_\perp=(n_\alpha\xi^2_{\alpha\beta}n_\beta)^{1/2}$. We chose here and in the following a coordinate system with the x axis perpendicular to the slab, and the boundaries at $x=0$ and $x=L$.

The transition temperature T_c is determined by the condition $\Psi(L+b_\perp)=0$, which gives for $L\gg\xi_\perp$

$$\frac{T_c}{T_c^0}=1-\pi^2\left(\frac{\xi_\perp}{L+2b_\perp}\right)^2. \tag{16}$$

The reduction in the transition temperature and the R dependence of the order parameter $\Psi(\vec{R})$ can be calculated for arbitrary slab sizes L, i.e., also for $L<\xi_\perp$, from the quasiclassical Eqs. (1)–(3). A comparison of these results with the GL results (13) and (16) allows us to determine the orientation-dependent extrapolation length $b_\perp$, and to deduce from it the surface-pair-breaking parameter $a(\vec{n})$. We will follow this route for calculating $a(\vec{n})$ in this paper. It should be emphasized that the $a(\vec{n})$, calculated for the simple slab geometry in the absence of a magnetic field, can be used in a GL theory for much more complex physical situations. An example would be a superconducting grain of

nontrivial geometry in a magnetic field, whose study by the full Fermi-liquid theory of superconductivity is feasible but difficult. The GL theory of such a grain, on the other hand, is a routine task for present day computers.

We start the quasiclassical theory of the slab by solving the transport equation (1). One obtains for an arbitrary $\Delta(\vec{p}_f,x)$ the solution

$$f^M(\vec{p}_f^{\,+},x;\epsilon_n)=\frac{2\pi}{\hbar|v_{fx}(p_f^+)|}\int_0^x dx'\ \exp[-\kappa^+(x-x')]\times\Delta(\vec{p}_f^{\,+},x')+F^+(\vec{p}_f^{\,+};\epsilon_n)\exp(-\kappa^+x) \tag{17}$$

for particles moving in the positive x direction and

$$f^M(\vec{p}_f^{\,-},x;\epsilon_n)=\frac{2\pi}{\hbar|v_{fx}(p_f^-)|}\int_x^L dx'\ \exp[\kappa^-(x-x')]\times\Delta(\vec{p}_f^{\,-},x')+F^-(\vec{p}_f^{\,-};\epsilon_n)\exp[\kappa^-(L-x)] \tag{18}$$

for particles moving in the negative x direction. We use the superscripts $+$ [$-$] for quasiparticles moving in the positive [negative] x direction, i.e., $v_{fx}(\vec{p}_f^{\,+})>0$ [$v_{fx}(\vec{p}_f^{\,-})<0$]. The exponential decay of the integrands depends on the Fermi velocities and the Matsubara energies, and is set by

$$\kappa^{\pm}=\frac{2\epsilon_n}{\hbar|v_{fx}(p_f^{\pm})|}. \tag{19}$$

The distinction between quasiparticles moving in positive and negative x directions is important for the boundary conditions at $x=0$ and $x=L$. Quasiparticles with momenta $\vec{p}_f^{\,+}$ ($\vec{p}_f^{\,-}$) are "outgoing" at $x=0$ and "incoming" at $x=L$ (and vice versa). The boundary condition (3) gives two coupled equations

$$F^+(\vec{p}_f^{\,+};\epsilon_n)=\int d^2p_f^-\ n(\vec{p}_f^{\,-})R(\vec{p}_f^{\,+},\vec{p}_f^{\,-})\times\left(\frac{2\pi}{\hbar|v_{fx}(p_f^-)|}\int_0^L dx'\ \exp(-\kappa^-x')\times\Delta(\vec{p}_f^{\,-},x')+F^-(\vec{p}_f^{\,-};\epsilon_n)\exp(-\kappa^-L)\right), \tag{20}$$

and

$$F^-(\vec{p}_f^{\,-};\epsilon_n)=\int d^2p_f^+\ n(\vec{p}_f^{\,+})R(\vec{p}_f^{\,-},\vec{p}_f^{\,+})\times\left(\frac{2\pi}{\hbar|v_{fx}(p_f^+)|}\int_0^L dx'\ \exp[-\kappa^+(L-x')]\times\Delta(\vec{p}_f^{\,+},x')+F^+(\vec{p}_f^{\,+};\epsilon_n)\exp(-\kappa^+L)\right), \tag{21}$$

which serve to pin down the two functions $F^+(\vec{p}_f^{\,-};\epsilon_n)$ and $F^-(\vec{p}_f^{\,-};\epsilon_n)$. These functions have a direct physical interpretation in the classical transport problem for quasiparticles. They describe the contributions to the distribution functions $f^M(\vec{p}_f,x;\epsilon_n)$ originating from reflections at the surfaces. The reflection term F^+ (F^-) describes the effect of the surfaces on right-moving (left-moving) quasiparticles. This interpretation can be inferred directly from Eqs. (17), (18). The two terms are coupled via Eqs. (20), (21). The surface-to-surface coupling is caused by multiple reflection at the two surfaces, and decreases exponentially for a large surface-to-surface separation L. This leads to the exponential factors $\propto\exp(-\kappa^{\pm}L)$ in the coupling terms in Eqs. (20), (21). For a large separation ($L\gg\xi_0$) the regions of distorted superconductivity near the left and right surfaces become decoupled.

A solution of Eqs. (20), (21) together with Eq. (7) determines the reflection terms as linear functions of the order parameter $\Psi(x)$. Insertion into Eqs. (17), (18) then gives us the distribution functions f^M in terms of $\Psi(x)$. This result can be used for eliminating f^M from the self-consistency equation (2) in favor of $\Psi(x)$. One ends up with a linear integral equation for $\Psi(x)$, whose kernel is de Gennes' kernel generalized to d-wave pairing. The integral equation will be used to calculate the GL extrapolation length and the transition temperature of a narrow slab. Analogous calculations for p-wave pairing in superfluid ^{3}He have been published in Refs. 31,32.

III. RESULTS

A. Model for layered d-wave superconductors

In order to proceed further one has to specify the various input material parameters in Eqs. (1), (2), and (3). These are the Fermi-surface data $\vec{p}_f$ and $\vec{v}_f$, the pairing interaction $V_{\rm BCS}$, and the reflection probabilities at the surface, $R(\vec{p}_f^{\,\rm out},\vec{p}_f^{\,\rm in})$. In the following we discuss the simplest model for a layered d-wave superconductor with a negligible small interlayer coupling. The Fermi surface shall be approximated by a single cylinder of radius p_f oriented along the c direction. The Fermi velocity in the c direction is zero in this model, and the layers are decoupled. It is convenient to parametrize the Fermi surface by cylindrical coordinates, i.e., the momentum in the c direction, p_{fz}, and the polar angle ϕ in the p_x-p_y plane. We will put the origin of the polar coordinates, $\phi=0$, in the x direction. This is the direction normal to the surfaces of the slab (see Fig. 1). The direction of the crystal a axis is, in general, rotated by an angle ϕ_0 with respect to the surface normal. The perpendicular momentum to the layers, p_{fz}, is unimportant in the model of decoupled layers, and can be dropped. Thus, the normalized Fermi-surface integrals are given in these coordinates by

$$\int d^2p_f\ n(\vec{p}_f)\cdots\rightarrow\int\frac{d\phi}{2\pi}\cdots. \tag{22}$$

We take the pairing interaction [Eq. (2)] as purely d wave of symmetry B_{1g};

$$V_{\rm BCS}(\phi,\phi')=2g\ \cos[2(\phi-\phi_0)]\cos[2(\phi'-\phi_0)], \tag{23}$$

where g is a dimensionless interaction constant. The maxima of the the gap are locked to the main crystal axes at $\phi=\pm\phi_0$ (a axis), and $\phi=\pm(\phi_0+\pi/2)$ (b axis).

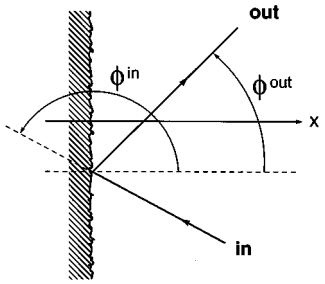

FIG. 1. Sketch of the classical trajectory of a quasiparticle approaching a rough wall along the incoming (in) part of the trajectory and being reflected into the outgoing (out) part. The angles ϕ^{in} and ϕ^{out} specify the directions of the Fermi velocity of the incoming and outgoing quasiparticles.

The simplest model for a surface with some degree of roughness is the Reuter-Sondheimer[33] model, in which a quasiparticle is reflected diffusely with probability p, and specularly with probability $1-p$:

$$R(\phi^{out},\phi^{in})=p\,\pi|\cos(\phi^{in})|+(1-p)2\pi\delta(\phi^{out}+\phi^{in}-\pi). \tag{24}$$

The model of Reuter and Sondheimer has one parameter, the diffusivity p.

The Fermi-surface data, pairing interaction, and surface model complete the list of material parameters for our calculations. They define what may be considered the simplest nontrivial model of a layered d-wave superconductor with weak interlayer coupling. The model has three relevant material parameters: (a) the coupling constant g which determines T_c^0 and will be eliminated in favor of T_c^0, (b) the Fermi velocity v_f which enters the coherence length $\xi_0=\hbar v_f/2\pi k_B T_c$ and will be absorbed into ξ_0, and (c) the roughness parameter p of the surface. The first two parameters disappear if we measure temperatures in units of T_c^0 and lengths in units of ξ_0. Hence, the remaining parameters of interest for our calculations are T/T_c^0, p, and the geometric parameters L/ξ_0 (slab width) and ϕ_0 (slab orientation).

B. Numerical calculations

We focus in our calculation on wide slabs ($L/\xi_0>1$) for which the coupling terms in Eqs. (20), (21) can be neglected. In this case, Eqs. (20), (21) can trivially be solved for F^+ and F^-. The result can be inserted into Eqs. (17), (18), and the resulting distribution functions f^M can be used to convert Eq. (2) into an equation for the microscopic order parameter $\Delta(\vec{p}_f,\vec{R})$. Equation (2) then turns, by using the translational invariance along the slab and the factorization,

$$\Delta(\vec{p}_f,\vec{R})=\Psi(x)\times\sqrt{2}\cos(\phi-\phi_0), \tag{25}$$

into an integral equation for $\Psi(x)$ of the form

$$\Psi(x)=g\int_0^L dx'\ \mathscr{K}_T^{\rm bulk}(x-x')\Psi(x')+g\int_0^L dx'\ \mathscr{K}_T^{(0)}\times(x,x')\Psi(x')+g\int_0^L dx'\ \mathscr{K}_T^{(L)}(x,x')\Psi(x'). \tag{26}$$

Equation (2), which determines the above kernels $\mathscr{K}_T^{\rm bulk}$, $\mathscr{K}_T^{(0)}$, and $\mathscr{K}_T^{(L)}$, requires summation over the Matsubara energies and a Fermi-surface integral. The Matsubara sum is a geometric series, and one is left with the following Fermi-surface integrals (ϕ integrals):

$$\mathscr{K}_T^{\rm bulk}(x-x')=\cos^2(2\phi_0)\int_{-\pi/2}^{\pi/2}\frac{d\phi}{2\pi}\frac{2T\,\cos^2(2\phi)}{\cos(\phi)\sinh\left(T\left|\frac{x-x'}{\cos(\phi)}\right|\right)}+\sin^2(2\phi_0)\int_{-\pi/2}^{\pi/2}\frac{d\phi}{2\pi}\frac{2T\,\sin^2(2\phi)}{\cos(\phi)\sinh\left(T\left|\frac{x-x'}{\cos(\phi)}\right|\right)}, \tag{27}$$

$$\mathscr{K}_T^{(0)}(x,x')=\frac{1-p}{2}[\cos(4\phi_0)+1]\int_{-\pi/2}^{\pi/2}\frac{d\phi}{2\pi}\frac{2T\,\cos^2(2\phi)}{\cos(\phi)\sinh\left(T\left|\frac{x+x'}{\cos(\phi)}\right|\right)}$$

$$+\frac{1-p}{2}[\cos(4\phi_0)-1]\int_{-\pi/2}^{\pi/2}\frac{d\phi}{2\pi}\frac{2T\,\sin^2(2\phi)}{\cos(\phi)\sinh\left(T\left|\frac{x+x'}{\cos(\phi)}\right|\right)}$$

$$+p\cos^2(2\phi_0)\int_{-\pi/2}^{\pi/2}\frac{d\phi^{out}}{2\pi}\int_{\pi/2}^{3\pi/2}\frac{d\phi^{in}}{2\pi}\frac{2\pi T\,\cos(2\phi^{out})\cos(2\phi^{in})}{\sinh\left[T\left(\left|\frac{x}{\cos(\phi^{out})}\right|+\left|\frac{x'}{\cos(\phi^{in})}\right|\right)\right]}, \tag{28}$$

$$\mathscr{K}_T^{(L)}(x,x') = \frac{1-p}{2}[\cos(4\phi_0)+1]\int_{-\pi/2}^{\pi/2}\frac{d\phi}{2\pi}\frac{2T\cos^2(2\phi)}{\cos(\phi)\sinh\left(T\left|\frac{2L-x-x'}{\cos(\phi)}\right|\right)}$$
$$+\frac{1-p}{2}[\cos(4\phi_0)-1]\int_{-\pi/2}^{\pi/2}\frac{d\phi}{2\pi}\frac{2T\sin^2(2\phi)}{\cos(\phi)\sinh\left(T\left|\frac{2L-x-x'}{\cos(\phi)}\right|\right)}$$
$$+p\cos^2(2\phi_0)\int_{-\pi/2}^{\pi/2}\frac{d\phi^{\rm in}}{2\pi}\int_{\pi/2}^{3\pi/2}\frac{d\phi^{\rm out}}{2\pi}\frac{2\pi T\cos(2\phi^{\rm in})\cos(2\phi^{\rm out})}{\sinh\left[T\left(\left|\frac{L-x}{\cos(\phi^{\rm in})}\right|+\left|\frac{L-x'}{\cos(\phi^{\rm out})}\right|\right)\right]}. \quad (29)$$

The bulk kernel $\mathscr{K}_T^{\rm bulk}$ derives from classical trajectories of excitations which do not hit the surfaces. The surface kernels $\mathscr{K}_T^{(0)}$ and $\mathscr{K}_T^{(L)}$ derive from classical trajectories of excitations which hit the surface at $x=0$ and $x=L$, respectively. The temperature T is measured in Eqs. (27)–(29) in units of T_c^0 and the lengths in units of ξ_0.

Equation (26) still contains the coupling constant g which must be eliminated in favor of the bulk transition temperature T_c^0. We do this by using the equation for the bulk transition temperature T_c^0

$$\frac{1}{g}=\int_{-\infty}^{+\infty}dx'\ \mathscr{K}_{T_c^0}^{\rm bulk}(x-x'), \quad (30)$$

where the kernel $\mathscr{K}_{T_c^0}^{\rm bulk}$ is obtained from Eq. (27) by setting $T=1$, i.e., to the bulk transition temperature. The elimination of g in Eq. (26) thus leads to our final equation for $\Psi(x)$:

$$\int_{-\infty}^{+\infty}dx'\ \mathscr{K}_{T_c^0}^{\rm bulk}(x-x')\Psi(x)$$
$$=\int_0^L dx'\ \mathscr{K}_T^{\rm bulk}(x-x')\Psi(x')+\int_0^L dx'\ \mathscr{K}_T^{(0)}$$
$$\times(x,x')\Psi(x')+\int_0^L dx'\ \mathscr{K}_T^{(L)}(x,x')\Psi(x'). \quad (31)$$

The elimination of g also eliminated a logarithmic singularity which plagues both Eqs. (26) and (30). The singularities cancel each other in Eq. (31), and it becomes free of divergences for $x-x'\to 0$. The linear integral equation (31) is thus in a form which admits a routine numerical solution. We first calculate the various kernels $\mathscr{K}^{\rm bulk}$, $\mathscr{K}^{(0)}$, and $\mathscr{K}^{(L)}$, defined in Eqs. (27), (28), (29), by standard integration routines, and then solve Eq. (31) by discretizing the integrals and using standard routines for finding eigenvalues and eigenvectors of the resulting homogeneous linear system.

C. Extrapolation length

In our Fermi-surface model the coherence-length tensor is diagonal, and the extrapolation-length tensor, introduced in Eq. (12), simplifies to

$$b(\phi_0)=\frac{\xi^2}{a(\vec{n})}, \quad (32)$$

where ξ^2 is the GL coherence length, and ϕ_0 measures the relative orientation of the axis of maximum gap and the surface normal. We determine $b(\phi_0)$ by calculating the amplitude $\Psi(x)$ of the microscopic order parameter near T_c for a slab of width L and orientation ϕ_0. The amplitude is defined by the relation

$$\Delta(x,\phi)=\Psi(x)\Delta_0(\phi), \quad (33)$$

where the anisotropic part of the microscopic order parameter is fixed in our model to $\Delta_0(\phi)=\sqrt{2}\cos[2(\phi-\phi_0)]$. For a wide slab this microscopic amplitude will agree away from the surfaces with the GL order parameter, and one obtains the extrapolation length by fitting the microscopic solution away from the surfaces to the GL solution (13). Figure 2 shows typical results for the amplitude $\Psi(x)$ in a slab of width $15\xi_0$ and specular surfaces. The d-wave order parameter is not affected by the surfaces for the ideal orientation $\phi_0=0°$, and maximum pair breaking occurs at $\phi=45°$. This result is a consequence of the very different behavior of the microscopic order parameter along reflected trajectories of

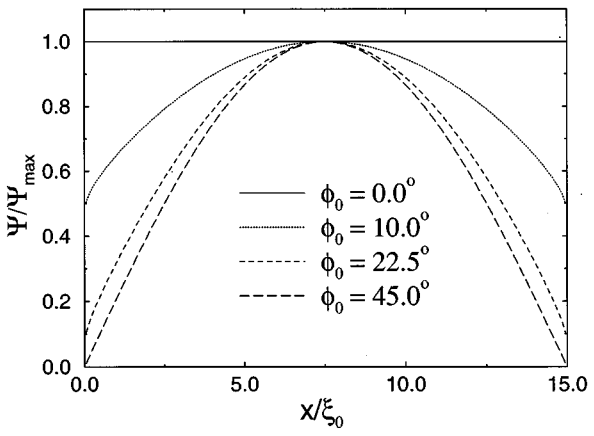

FIG. 2. Spatial variation of the order parameter of a d-wave superconductor in a slab of width $15\xi_0$ with smooth ($p=0$) boundaries. The depletion of the order parameter near the boundaries depends on the relative orientation angle ϕ_0 of the surface and the crystal lattice.

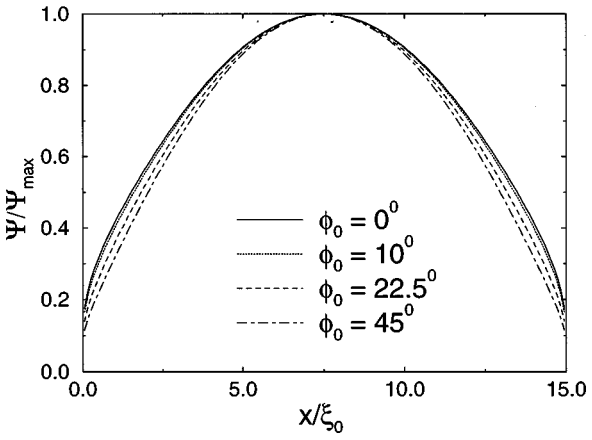

FIG. 3. Same as Fig. 2, but for a slab with rough ($p=1$) boundaries.

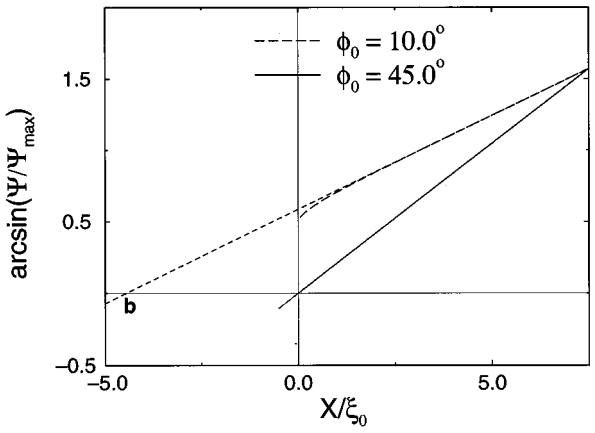

FIG. 4. The function $\arcsin[\Psi(x)/\Psi_{max}]$ is used to extract the extrapolation length b from the order parameter in a slab. This arcsine function is linear in the region of validity of the GL theory, and the extrapolation of the linear part determines the extrapolation length. We display typical examples for a slab with smooth walls and two orientation angles. The order parameters $\Psi(x)$ are shown in Fig. 2. The extrapolation length is zero for the orientation angle of maximal pair breaking ($\phi_0=45°$), infinity for $\phi_0=0°$ (not shown), and $\approx 4.5\xi_0$ for the intermediate orientation angle $\phi_0=10°$.

quasiparticles. For $\phi_0=0$ the order parameter along an incoming trajectory is the same as along the outgoing one (constructive trajectory), i.e., $\Delta_0(\phi^{out})=\Delta_0(\phi^{in})$. Consequently, the contribution of a reflected trajectory in the slab is the same as that of a straight trajectory with direction ϕ^{in} in a bulk sample, and there is no pair breaking at these surfaces. In the second case, on the other hand, the microscopic order parameter flips sign along a reflected trajectory because $\Delta_0(\phi^{out})=-\Delta_0(\phi^{in})$. The reflected trajectories contribute negatively to the kernel, and are strongly pair breaking (destructive trajectory). This strong pair breaking effect is a consequence of the microscopic order parameter changing sign in a reflection at the (110) plane. This effect will not occur for anisotropic s-wave superconductors with no sign change, or only small regions on the Fermi surface with an order parameter of different sign. Results for the order parameter of a slab with rough surfaces are shown in Fig. 3. Constructive and destructive trajectories are always mixed at a rough surface, independent of its orientation, and one finds an intermediate extrapolation length of the order ξ_0.

A comparison of the microscopic solution and the GL solution (a sine function) is shown in Fig. 4. The plot shows the arcsine of the microscopic amplitude, which would give straight lines for a pure sine function. The figure demonstrates the good fit to the GL solution in the interior of the slab and the deviations near the surface. The extrapolation of the straight line determines the extrapolation length (see Fig. 4). Formally, the extrapolation length of the GL theory is obtained from the microscopic calculations in the limit of an infinitely wide slab. Our calculations are done for finite slabs, and we show in Fig. 5 the dependence of the extrapolation length on the width L of the slab. These results approach the GL extrapolation length $b(\phi_0)$ for $L\to\infty$, and the deviations at finite L give estimates of the accuracy of the GL theory for slabs of finite thickness.

Our main results are given in Figs. 6 and 7. Figure 6 shows the calculated dependence of the extrapolation length on the orientation and roughness of the surface. The extrapolation length depends strongly on the surface-to-lattice orientation for perfectly reflecting surfaces ($p=0$). It ranges here from 0 to ∞. Any roughness weakens this strong sensitivity to the orientation, and only a small anisotropy is left for a rough surface. Figure 7 shows our results for the reduction in T_c in slabs of d-wave superconductors of thickness L. The amount of reduction depends on the orientation of the slab with respect to the crystal axes and on the surface quality. A slab with specular walls shows for $\phi_0=45°$ (orientation of strong pair breaking) a jump to $T_c=0$ at a critical thickness L_c. The critical thickness and the jump decrease with increasing roughness. A rough slab still has a finite L_c but T_c seems to approach zero continuously at L_c. No significant differences between different orientations of the surface are

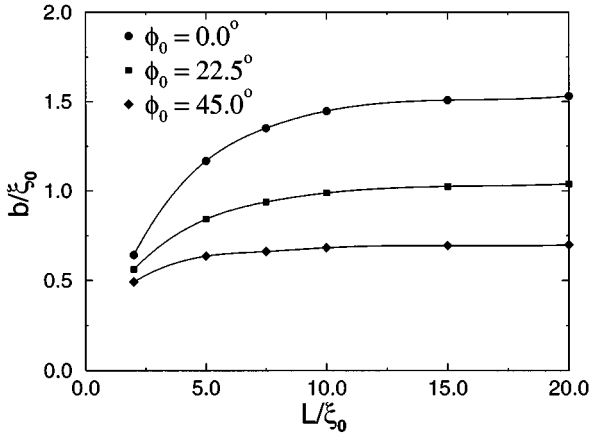

FIG. 5. Dependence of the extrapolation length on the width L of the slab. The true GL extrapolation length is obtained in the limit $L\to\infty$. The L dependence of the extrapolation length has no direct physical meaning. The shown deviations of b from the GL extrapolation length give an estimate for the error in a GL calculation for systems of finite size L. At $L=15\xi_0$, e.g., the error is below 10%.

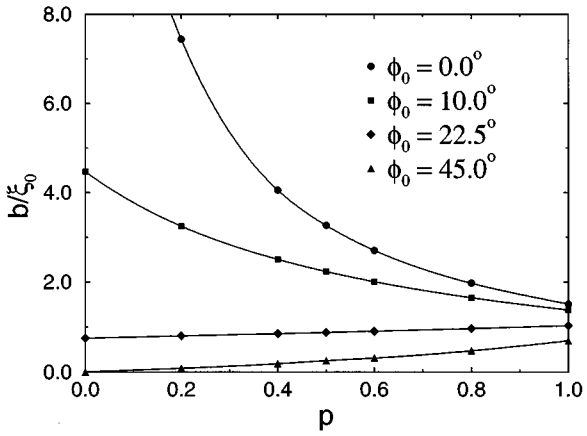

FIG. 6. Dependence of the GL extrapolation length b on the surface roughness p. Results are shown for the model d-wave superconductor, and several surface-to-lattice orientation angles ϕ_0. A very strong dependence of b on the orientation angle is obtained for smooth surfaces ($p \ll 1$).

found for rough ($p=1$) surfaces, as shown in Fig. 7. It should be noted that increasing roughness increases the pair breaking effect for the $\phi_0=0°$ orientation, whereas it reduces the pair breaking effect for the $\phi_0=45°$ orientation. Specular reflection at a 45° surface leads to a sign change for all trajectories, and thus to a maximal pair breaking. Random scattering at the surfaces mixes in less destructive trajectories (e.g., with no sign change), and thus reduces the surface pair

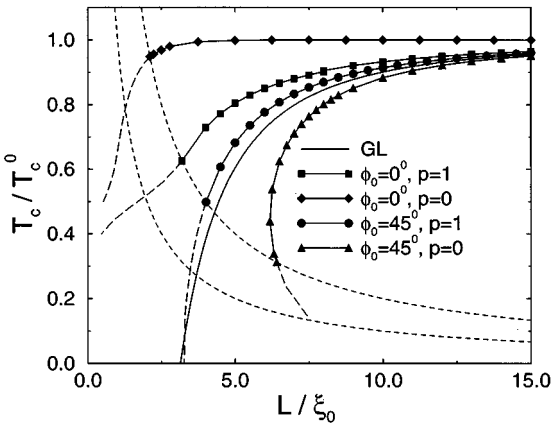

FIG. 7. Critical temperature of a d-wave superconductor as function of the width of the slab. The marked curves show results for smooth surfaces ($p=0$), rough surfaces ($p=1$), and two different surface to lattice orientation angles. The solid line is shown for comparison. It represents the result of the GL theory for an extrapolation length $b=0$. The calculations use the wide-channel approximation $L \gg \xi_{Tc}$, where ξ_{Tc} is the effective coherence length at the transition temperature of the slab, $\xi_{Tc}=\xi_0 T_c^0/T_c$. The two dashed lines show the location of the curves $L=\xi_{Tc}$ (left line) and $L=2\xi_{Tc}$ (right line). This indicates roughly the dividing line at which our approximation breaks down. Calculated results beyond the right dividing line are shown as dashed continuations of the solid lines. The breakdown of the wide-channel approximation is clearly seen for the slab with optimal orientation $\phi_0=0$ and ideal surfaces $p=1$. The exact result is $T_c/T_c^0=1$, and the approximate result starts deviating from the exact one at about $L/\xi_{Tc}=2$.

breaking. Just the opposite situation holds for a 0° surface. Specularly reflected trajectories are not pair breaking, and roughness mixes in pair breaking trajectories.

IV. SUMMARY

In view of the ongoing discussion of both the symmetry of the condensed pairs and the proper theory of high-T_c superconductors, it is desirable to measure properties which carry information on the pairing symmetry, and which can be analyzed by a quantitative theory of superconductivity. The Ginzburg-Landau (GL) theory provides a powerful tool for analyzing the effects of d-wave pairing on the superconducting properties. In particular, the surface and interface terms of the GL theory show important qualitative, as well as quantitative, differences between s-wave and d-wave pairing in tetragonal crystals.

In this work we study the GL theory of d-wave superconductors near surfaces. The boundary condition for the order parameter of the phenomenological GL equation is formulated in terms of an ''extrapolation length'' of the order parameter at the surface. One purpose of this work is to develop the theory of the extrapolation length for an anisotropic superconductor with an anisotropic Fermi surface and anisotropic pairing amplitude. A second purpose is to demonstrate that sizable quantitative differences in the magnitude and anisotropy of the extrapolation length are expected for d-wave and (anisotropic) s-wave superconductors. We calculate the kernel to the linearized gap equation using de Gennes' method as developed for p-wave superconductors, and derive from it the dependence of the extrapolation length on the surface orientation and the degree of surface roughness. The most pronounced effects of d-wave pairing on the GL boundary condition are expected for smooth surfaces (specular reflection). One finds a large difference in the extrapolation length for (100) and (010) surfaces, which have an infinite extrapolation length, versus (110) surfaces, which have an extrapolation length $\approx \xi_0$. This result follows directly from symmetry arguments, as first shown in Ref. 31. The anisotropy is diminished to some degree with increasing roughness of the surface. Effects which measure these anisotropies are, for instance, the reduction in T_c in narrow geometries (size effect), the surface critical field H_{c3}, tunneling, and other surface sensitive probes. We present detailed results for the depression of T_c in narrow slabs, which might be observed in strips of cuprate superconductors with their long axis in the a-b plane.

After completing this work we became aware of a manuscript by Barash, Galaktionov, and Zaikin.[34] The authors discuss in Sec. II the extrapolation length at specular surfaces of d-wave superconductors with spherical Fermi surfaces. These results are fully equivalent to our results for superconductors with cylindrical Fermi surfaces in the limit $p=0$.

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