Virial theorem and Abrikosov's solution of the Ginzburg-Landau equations

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Using the virial theorem discovered recently by Doria, Gubernatis, and Rainer [Phys. Rev. B **39**, 9573 (1989)], we rederive Abrikosov's solution of the Ginzburg-Landau equations near H_{c2} in a very simple way. We stress the importance of the virial theorem for an intuitive understanding of the vortex state and report a generalized version of it, which is valid within the framework of the quasiclassical theory of superconductivity.

I. INTRODUCTION

The following remarkable relation has recently been derived for a superconductor in the mixed state by Doria, Gubernatis, and Rainer[1] using the invariance of the Ginzburg-Landau (GL) free energy under an appropriate scaling transformation:

$$\mathbf{H}\cdot\mathbf{B}=4\pi(F_{\text{kin}}+2F_{\text{field}}) \; . \tag{1}$$

Here **H** is the external field, **B** the macroscopic induction, and F_{kin} and F_{field} denote the kinetic-energy term and the field energy term of the GL free energy, respectively (if not stated otherwise, we use in this Brief Report the notation of Ref. 2). Equation (1) has been termed a "virial theorem" because it is a consequence of the same invariance principle that leads to the standard virial theorem of classical mechanics. Another essential point entering the derivation of Eq. (1) is the quantization of magnetic flux in the superconducting state. It is astonishing that a relation as simple and fundamental as Eq. (1) has not been discovered during so many years of theoretical work on the GL equations of superconductivity.

As pointed out in Ref. 1, Eq. (1) defines the relation **H**(**B**) in a relatively straightforward manner. The fields entering the right-hand side (rhs) of Eq. (1) have to be calculated for a fixed value of the induction **B**. The associated external field **H**, belonging to this fixed value of **B**, is then directly given by Eq. (1). This fact presents an important potential application of the virial theorem. Up to now, one had to calculate—either analytically or numerically with a sufficient degree of accuracy—the *complete* induction dependence of the free energy F in order to obtain the required relation **H**(**B**) from the derivative of F with respect to **B**. Consequently, the importance of Eq. (1) for numerical studies on type-II superconductors has been stressed in Ref. 1.

The general purpose of the present work is to point out that the virial theorem may be useful in several other respects as well. We first show, in the remaining part of the Introduction, that the virial theorem leads naturally to the notion of a field $H_c(\mathbf{x})$, which may be considered as a spatially varying generalization of the thermodynamic critical field H_c. In our opinion, this notion might be useful for our intuitive understanding of the mixed state. In Sec. II we present the (generalized) virial theorem of the quasiclassical theory of superconductivity. As an example for the usefulness of the virial theorem in analytical calculations we report in Sec. III a very simple derivation of Abrikosov's fundamental identities, which constitute the main part of his famous solution[3,4] of the GL equations near the upper critical field H_{c2}. Section IV is devoted to conclusions.

The quantities F_{kin} and F_{field}, referred to in Eq. (1), are given by

$$F_{\text{kin}}=\frac{1}{V}\int d^3x\frac{1}{2m^*}\left|\left[\frac{\hbar}{i}\nabla-\frac{2e}{c}\mathbf{A}\right]\Delta(\mathbf{x})\right|^2 , \tag{2}$$

$$F_{\text{field}}=\frac{1}{V}\int d^3x\frac{1}{8\pi}\mathbf{B}^2(\mathbf{x}) \; . \tag{3}$$

The complete Helmholtz free energy of GL theory is then given by

$$F=-F_{\text{cond}}+F_{\text{kin}}+F_{\text{field}} \tag{4}$$

with the condensation energy F_{cond} defined by

$$F_{\text{cond}}=-\frac{1}{V}\int d^3x\left[\alpha|\Delta(\mathbf{x})|^2+\frac{\beta}{2}|\Delta(\mathbf{x})|^4\right] . \tag{5}$$

Inserting Eq. (1) into the Ginzburg-Landau Gibbs free energy G, which is given by

$$G=F-\frac{1}{4\pi}\mathbf{HB} \; , \tag{6}$$

one obtains $G=-F_{\text{cond}}-F_{\text{field}}$, or

$$G=\frac{1}{V}\int d^3x\left[-\frac{H_c^2(\mathbf{x})}{8\pi}-\frac{\mathbf{B}(\mathbf{x})^2}{8\pi}\right] , \tag{7}$$

where a spatially dependent field $H_c(\mathbf{x})$, defined by

$$-\frac{H_c^2(\mathbf{x})}{8\pi}=\alpha|\Delta(\mathbf{x})|^2+\frac{\beta}{2}|\Delta(\mathbf{x})|^4 \tag{8}$$

has been introduced.

The Gibbs free energy of the mixed state as given by Eq. (7) takes a very simple form which, to our knowledge, has never been reported prior to Ref. 1. The appealing feature of Eq. (7) is that it consists of two well-defined terms which both have a simple physical meaning (and a well-known qualitative behavior). The Gibbs free-energy difference between the homogeneous (Meissner) superconducting state and the normal state is given by $-H_c^2/8\pi+H^2/8\pi$. Equation (7) shows that the factor $-H_c^2/8\pi$, which favors the superconducting state, is split in the mixed state into two parts (both favoring superconductivity); a magnetic field energy and a spatially varying condensation energy, defined by Eq. (8). In contrast to the approximate way the notion of condensation energy is commonly used, when applied to a spatially inhomogeneous situation (a well-known example is "condensation energy pinning" of flux lines by normal conducting inclusions), Eqs. (7) and (8) now give a precise meaning to this term.

One can try to improve our understanding of the mixed state with the help of the local quantity $H_c^2(\mathbf{x})/8\pi$ [$H_c(\mathbf{x})$ playing the role of a local thermodynamic field]; when doing so, it should be borne in mind that thermodynamic equilibrium is still determined by averaged values of the local quantities. Of course, a quantitative knowledge of the Gibbs free-energy density $g(\mathbf{x})$, as given by Eq. (7), still requires solving the coupled GL equations. However, since the qualitative behavior of the fields entering Eq. (7) is known, it now becomes—without contributions of unknown behavior, from gradient (and other) terms—simpler to understand the interplay between magnetic field energy and condensation energy near a flux line. We mention, without going into details, that the decrease of the magnetic field $B(0)$, at the center of an isolated flux line, with increasing GL parameter κ is one of the qualitative results which can be read off immediately from Eq. (7). Another example is the relation $[\mathbf{B}(\mathbf{x})/H_c]^2=(1-|\psi(\mathbf{x})|^2)^2$ [here, the order parameter ψ is measured in units of $(-\alpha/\beta)^{1/2}$], which holds at $\kappa=1/\sqrt{2}$ and $H=H_c$, where $g(\mathbf{x})$ is *locally* equal to its Meissner state value.

II. VIRIAL THEOREM OF THE QUASICLASSICAL THEORY

An appropriate theoretical framework for a quantitative description of superconductors well below T_c is given by the quasiclassical or Eilenberger equations.[5,6] The variables to be determined in this theory are the order parameter Δ, the vector potential $\mathbf{A}$ and, in addition, the Green's functions f, $f^\dagger$ and g. A free-energy functional whose stationarity conditions lead to the quasiclassical equations has been constructed by Eilenberger.[5] It may be written in the form

$$F=F_{\text{field}}+F_{\text{grad}}+F_{\text{ord}}+F_{\text{imp}} . \quad (9)$$

Here, F_{field} is defined by Eq. (3). The term F_{grad}, containing first-order derivatives of f and $f^\dagger$, is given by

$$F_{\text{grad}}=\frac{1}{V}\int d^3\mathbf{x}\frac{2\pi}{\hbar\beta}N(0)\times\sum_{l=0}^{\infty}\int d^2\mathbf{k}\,\rho(\mathbf{k})g\mathbf{v}(\mathbf{k})\times\left[\frac{\hbar}{2}\nabla\ln(f/f^\dagger)-i\frac{2e}{c}\mathbf{A}\right] , \quad (10)$$

the term F_{imp}, describing scattering at nonmagnetic impurities, is given by

$$F_{\text{imp}}=\frac{1}{V}\int d^3\mathbf{x}\frac{2\pi}{\hbar\beta}N(0)\sum_{l=0}^{\infty}\int d^2\mathbf{k}\rho(\mathbf{k})\tfrac{1}{2}\int d^2\mathbf{q}\,\rho(\mathbf{q})W(\mathbf{k},\mathbf{q})[\tfrac{1}{2}f^\dagger(\mathbf{k})f(\mathbf{q})+\tfrac{1}{2}f(\mathbf{k})f^\dagger(\mathbf{q})+g(\mathbf{k})g(\mathbf{q})-1] , \quad (11)$$

and the remaining part of the free energy, denoted somewhat arbitrarily by F_{ord}, is given by

$$F_{\text{ord}}=\frac{1}{V}\int d^3\mathbf{x}\left[N(0)\left[\ln(T/T_c)+\frac{2\pi}{\hbar\beta}\sum_{l=0}^{\infty}\omega_l^{-1}\right]|\Delta|^2+\frac{2\pi}{\hbar\beta}N(0)\sum_{l=0}^{\infty}\int d^2\mathbf{k}\,\rho(\mathbf{k})[\Delta f^\dagger+\Delta^* f+2\omega_l(g-1)]\right] . \quad (12)$$

Eilenberger's free energy is stationary with respect to variations of Δ, $\mathbf{A}$, f, and $f^\dagger$ but not of g; in Eqs. (10)–(12) the quantity g is to be understood as an abbreviation for $(1-ff^\dagger)^{1/2}$. The Green's functions depend on the spatial coordinate $\mathbf{x}$, on the quasiparticle wave vector $\mathbf{k}$, and on the Matsubara frequency ω_l. Not all of these variables are written down explicitly in Eqs. (10)–(12). For all other details of notation used in Eqs. (10)–(12), the reader is referred to the original article by Eilenberger.[5]

In GL theory, a translation along each one of the primitive vectors $\mathbf{b}_i$ of the unit cell of the flux-line lattice can be written as a gauge transformation of the variables $\mathbf{A}$ and Δ:

$$\mathbf{A}(\mathbf{x}+\mathbf{b}_i)=\mathbf{A}(\mathbf{x})+\nabla\chi_i(\mathbf{x}) , \quad (13)$$

$$\Delta(\mathbf{x}+\mathbf{b}_i)=\Delta(\mathbf{x})\exp\left[i\frac{2e}{\hbar c}\chi_i(\mathbf{x})\right] . \quad (14)$$

Equations (13) and (14) are the (periodic) boundary conditions for the GL equations when applied to the mixed state.

The basic point in the derivation of the virial theorem of the GL theory was to show that the periodic boundary conditions of the GL equations determine the averaged magnetic field B in a unique way.[1] It is an easy matter, and will not be repeated here, to show that the same is true in the quasiclassical theory. We note that, in this theory, the above equations (13) and (14) remain valid (they have to be supplemented by gauge transformations[7,8] of f and $f^{\dagger}$). The periodic boundary conditions of the quasiclassical theory have recently been extensively used in numerical calculations.[7,8]

The remaining steps in the derivation of a quasiclassical virial theorem are also completely analogous to the derivation reported in Ref. 1. One performs a scaling transformation

$$\mathbf{x}'=\mathbf{x}/\lambda \ , \tag{15}$$

$$\Delta'(\mathbf{x}')=\Delta(\mathbf{x}'\lambda) \ , \quad \mathbf{A}'(\mathbf{x}')=\lambda\,\mathbf{A}(\mathbf{x}'\lambda) \ , \tag{16}$$

$$\begin{aligned} &f'(\mathbf{x}',\mathbf{k},\omega)=f(\mathbf{x}'\lambda,\mathbf{k},\omega) \ , \\ &f^{\dagger\prime}(\mathbf{x}',\mathbf{k},\omega)=f^{\dagger}(\mathbf{x}'\lambda,\mathbf{k},\omega) \ , \end{aligned} \tag{17}$$

and differentiates the free energy F—expressed in terms of the new variables—with respect to λ. The dependence of F on the boundary conditions must be taken into account. These boundary conditions are changed by the above scaling transformation. The λ dependence of F implied by the changing boundary conditions may be expressed in terms of a dependence of F on the scaled induction. The latter is given by

$$\mathbf{B}'=\lambda^2\mathbf{B} \ . \tag{18}$$

Setting $\lambda=1$ and using the thermodynamic relation

$$\mathbf{H}=4\pi\frac{\partial F}{\partial \mathbf{B}} \ , \tag{19}$$

one obtains, as a final result, the relation

$$\mathbf{H}\cdot\mathbf{B}=4\pi(\tfrac{1}{2}F_{\text{grad}}+2F_{\text{field}}) \ , \tag{20}$$

which is the virial theorem of the quasiclassical theory. Near T_c, the term $F_{\text{grad}}/2$ reduces to the GL term F_{kin}. Clearly, the numerical effort required to obtain a vortex-lattice solution of the quasiclassical equations is rather large.[7–9] Consequently, the virial theorem should be particularly useful in simplifying such calculations.

III. A SIMPLE DERIVATION OF ABRIKOSOV'S IDENTITIES

An essential part of Abrikosov's celebrated solution[3,4] of the GL equations consists in the derivation of two identities which also bear his name. With the help of these two fundamental identities,[4] one immediately obtains, apart from the remaining task of determining the geometrical constant β (see below), the desired solutions for the magnetization and the free energy near H_{c2}. In this section we show that Abrikosov's identities may be derived with the help of the virial theorem with much less mathematical effort than required by the usual derivations.[3,4]

The virial theorem, Eq. (1), may be simplified further with the help of the well-known identity

$$\frac{1}{V}\int d^3x\frac{1}{2m^*}\left|\left[\frac{\hbar}{i}\nabla-\frac{2e}{c}\mathbf{A}\right]\Delta(\mathbf{x})\right|^2 = -\frac{1}{V}\int d^3x[\alpha|\Delta(\mathbf{x})|^2+\beta|\Delta(\mathbf{x})|^4] \ , \tag{21}$$

which holds for solutions of the GL equations fulfilling the boundary condition

$$\mathbf{n}\left[\frac{\hbar}{i}\nabla-\frac{2e}{c}\mathbf{A}\right]\Delta(\mathbf{x})=0 \tag{22}$$

at the surface ($\mathbf{n}$ is the vector normal to the surface) of the considered volume. Equation (21) may be derived in a straightforward manner from the first GL equation by means of a partial integration.[4] For the present vortex-lattice solutions, Eq. (22) is clearly fulfilled. Using Eq. (21), the viral theorem (1) takes the form

$$\mathbf{H}\cdot\mathbf{B}=\frac{4\pi}{V}\int d^3x\left[-\alpha|\Delta(\mathbf{x})|^2-\beta|\Delta(\mathbf{x})|^4+\frac{\mathbf{B}(\mathbf{x})^2}{4\pi}\right] . \tag{23}$$

Now, the relation between the induction and the applied field near H_{c2} may be calculated by means of a very simple perturbation expansion. We write $B(\mathbf{x})=H-\phi(\mathbf{x})$, $H=H_{c2}-(H_{c2}-H)$, and assume that $\phi(\mathbf{x})$ and $H-H_{c2}$ are small, of order $[\Delta(\mathbf{x})]^2$, where $\Delta(\mathbf{x})$ is a solution of the (linearized) GL equation near H_{c2}. Inserting these expansions into Eq. (23) and selecting terms of order Δ^2 and Δ^4, one obtains, after a short calculation, the two desired relations

$$B=H-\frac{1}{2\kappa}\overline{|\psi(\mathbf{x})|^2} \tag{24}$$

and

$$\frac{H-\kappa}{\kappa}\overline{|\psi(\mathbf{x})|^2}+\left[1-\frac{1}{2\kappa^2}\right]\overline{|\psi(\mathbf{x})|^4}=0 \tag{25}$$

first found by Abrikosov[3] by means of much more involved computations. In Eqs. (24) and (25) and below, magnetic fields are measured in units of $\sqrt{2}H_c$ and the order parameter ψ is measured in units of $(-\alpha/\beta)^{1/2}$. The overbar denotes spatial averaging and B is the macroscopic induction. In deriving Eq. (25), Abrikosov's first identity, i.e., Eq. (24) without spatial averaging, has been used. Equation (24) is equivalent to a local relation, which one obtains from Abrikosov's first identity by adding an unknown function $\eta(\mathbf{x})$ fulfilling $\overline{\eta}=0$. We set $\eta(\mathbf{x})$ equal to zero since a nonzero value of η can be easily shown to yield an induction curve with an infinite slope at a value of κ different from $1/\sqrt{2}$ (the value of κ separating type-I from type-II behavior).

For completeness, we quote Abrikosov's final expression for the magnetic induction near the upper critical field,

$$B=H-\frac{\kappa-H}{(2\kappa^2-1)}\frac{1}{\beta} \ , \tag{26}$$

which may easily be obtained from the above relations. The numerical value of the geometrical constant β, defined by

$$\beta=\overline{|\psi(\mathbf{x})|^4}/\overline{|\psi(\mathbf{x})|^2}^2 \ , \tag{27}$$

cannot, of course, be obtained by means of the present simple approach (the result[4] for a triangular vortex lattice is $\beta=1.16$). Finally, we mention that Abrikosov's expression for the Gibbs free-energy difference (measured in units of $H_c^2/8\pi$) between the mixed state and the normal state,

$$G-G_n=-\frac{2(H-\kappa)^2}{(2\kappa^2-1)\beta}\ , \tag{28}$$

can also be derived with the help of the virial theorem, by using Eqs. (7), (24), and (25). The possibility that the virial theorem might be useful in other analytical calculations as well, should be taken into account.

IV. CONCLUSIONS

In this report we derived a quasiclassical version of the virial theorem of superconductivity valid for arbitrary temperature. By means of this relation, one should be able to achieve a considerable reduction of the computational effort required for microscopic calculations of thermodynamic quantities. Secondly, we demonstrated the usefulness of the virial theorem in analytical calculations by reporting a very simple derivation of Abrikosov's solution of the GL equations near the upper critical field. Most likely, the range of potential applications of the virial theorem in analytical calculations is not exhausted by the particular example reported here.

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