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Brief Reports

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Virial theorem for Ginzburg-Landau theories with potential applications to numerical studies of type-II superconductors

M. M. Doria
Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

J. E. Gubernatis
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

D. Rainer
Physikalisches Institut, Universität Bayreuth, D-8580 Bayreuth, Federal Republic of Germany
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In the framework of the Ginzburg-Landau theory, we derive and discuss the relation $\mathbf{H}\cdot\mathbf{B}=4\pi(F_{\text{kin}}+2F_{\text{field}}-\frac{1}{2}F_{\text{inhom}})$, which should be useful in numerical calculations of magnetic properties of type-II superconductors.

I. INTRODUCTION

In this Report we derive the following identity:

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

which holds in the Ginzburg-Landau approximation for a superconductor in a homogeneous external magnetic field $\mathbf{H}$. This identity relates the external field, the average magnetic field

$$\mathbf{B}=\frac{1}{V}\int d^3x\,\mathbf{B}(\mathbf{x})\,, \tag{2}$$

the average kinetic energy

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

and the average field energy

$$F_{\text{field}}=\frac{1}{V}\int d^3x\frac{1}{8\pi}\mathbf{B}^2(\mathbf{x})\,. \tag{4}$$

The term F_{inhom} is nonzero only for inhomogeneous systems with position-dependent material parameters and will be discussed at the end of Sec. II. The total microscopic field $\mathbf{B}(\mathbf{x})$ includes the externally applied field and the field generated by supercurrents.

Our relation (1) can be considered as a virial theorem in the sense that it as well as the standard virial theorem[1] are a consequence of invariances under a transformation of the length scale. The relation is probably of no practical use for the interpretation of experiments but can be a helpful tool for calculating magnetic properties of type-II superconductors. In fact, we discovered this theorem while trying to improve the accuracy of the numerical calculation of the magnetization curves of inhomogeneous superconductors.[2]

Before deriving Eq. (1) we will first review some basic facts of the Ginzburg-Landau theory that will be important. We start from the Ginzburg-Landau free energy

$$\Delta F=\frac{1}{V}\int d^3x\left[\alpha\,|\Delta(\mathbf{x})|^2+\frac{\beta}{2}\,|\Delta(\mathbf{x})|^4+\frac{1}{2m^*}\left|\left(\frac{\hbar}{i}\nabla-\frac{2e}{c}\mathbf{A}\right)\Delta(\mathbf{x})\right|^2+\frac{1}{8\pi}[\text{curl}\mathbf{A}(\mathbf{x})]^2\right]. \tag{5}$$

Variation of ΔF with respect to the fields $\Delta(\mathbf{x})$ and $\mathbf{A}(\mathbf{x})$ leads to the Ginzburg-Landau equation and the equation for the supercurrent. We will not need these equations in the following and refer the reader to standard textbooks[3] for notation and details. Obviously, the absolute minimum of the free energy (5) is the field-free state, $\mathbf{B}\equiv\text{curl}\mathbf{A}=0$, which is not of interest here. In order to describe a superconductor in the presence of an external field, one has to abandon the unrestricted minimization of (5) and impose constraints on the fields Δ and $\mathbf{A}$. We use the constraint of fixing the average magnetic field $\mathbf{B}$. The constrained minimum of ΔF is now a function of $\mathbf{B}$, and standard thermodynamic arguments yield the external field as the derivative of ΔF with respect to $\mathbf{B}$,

$$\mathbf{H}=4\pi\frac{\partial\Delta F}{\partial\mathbf{B}}\,. \tag{6}$$

The vector notation in (6) is unconventional but self-explaining.

In the following we implement the averaged magnetic field by imposing what will be called "periodic boundary conditions." In a perfect, infinite, type-II superconductor these boundary conditions fix the lattice parameters of the vortex lattice and lead to Abrikosov's vortex state.[4] On the other hand, one can also use this boundary condition for nonperfect, nonperiodic superconductors with, for example, normal-metal inclusions, grain boundaries, inhomogeneities in the chemical composition, or other defects. In this case, the unit cell of our periodic lattice must be interpreted as an artificial supercell, chosen large enough such that the defect superstructure has no significant physical consequences. We can finally let the size of the supercell go to infinity in order to eliminate these artifacts. The periodic boundary conditions for $\mathbf{A}$ and Δ have the form

$$\mathbf{A}(\mathbf{x}+\mathbf{b}_\nu)=\mathbf{A}(\mathbf{x})+\nabla\chi_\nu(\mathbf{x})\,, \tag{7a}$$

$$\Delta(\mathbf{x}+\mathbf{b}_\nu)=\Delta(\mathbf{x})\exp\left[i\frac{2e}{\hbar c}\chi_\nu(\mathbf{x})\right], \tag{7b}$$

and depend on the lattice structure, characterized by the set of lattice vectors $\mathbf{b}_\nu$, and on gauge potentials $\chi_\nu(\mathbf{x})$ associated with each $\mathbf{b}_\nu$. The conditions (7) mean that a translation by a lattice vector amounts to a gauge transformation or, in other words, that the fields $\mathbf{A}$ and Δ are invariant under lattice translations combined with specific gauge transformations. Consequently, all gauge-invariant quantities, such as $\mathbf{B}(\mathbf{x})$ or $|\Delta(\mathbf{x})|$, are periodic. The gauge potentials $\chi_\nu(\mathbf{x})$ cannot be chosen freely but must preserve the single valuedness of $\mathbf{A}$ and Δ, which implies the quantization of the magnetic flux. The single valuedness of Δ when circling along the edges of a face of a unit cell requires

$$\frac{2e}{\hbar c}[\chi_\alpha(\mathbf{x})+\chi_\beta(\mathbf{x}+\mathbf{b}_\alpha)-\chi_\alpha(\mathbf{x}+\mathbf{b}_\beta)-\chi_\beta(\mathbf{x})]=-2\pi N_{\alpha\beta}\,, \tag{8}$$

where $N_{\alpha\beta}$ is an integer and $\mathbf{b}_{\alpha,\beta}$ are the vectors spanning the face of the cell. Equation (7) together with (8) yields the flux through this face quantized in units of the flux quantum $\Phi_0=2\pi\hbar c/2e$:

$$\Phi_{\alpha\beta}\equiv\int\mathbf{A}\cdot d\mathbf{x}=N_{\alpha\beta}\Phi_0\,. \tag{9}$$

The quantum numbers $N_{\alpha\beta}=-N_{\beta\alpha}$ also determine the average magnetic field. By averaging $\mathbf{B}$ over a unit cell one finds

$$\mathbf{B}=\tfrac{1}{2}N_{\alpha\beta}\epsilon_{\alpha\beta\gamma}\mathbf{b}_\gamma\Phi_0/V\,, \tag{10}$$

where $\mathbf{b}_\gamma$ are three primitive vectors of the lattice and V is the volume of the unit cell. Relation (10) is important since it verifies that the periodic boundary conditions indeed fix the average magnetic field.

II. DERIVATION OF THE VIRIAL THEOREM

We are now in a position to derive our identity (1). We first change the length scale by a factor λ,

$$\mathbf{x}'=\mathbf{x}/\lambda\,, \tag{11}$$

and introduce a transformed order parameter and vector potential:

$$\Delta_\lambda(\mathbf{x}')=\Delta(\lambda\mathbf{x}')\,, \tag{12}$$

and

$$\mathbf{A}_\lambda(\mathbf{x}')=\lambda\mathbf{A}(\lambda\mathbf{x}')\,. \tag{13}$$

In the following, derivatives with respect to $\mathbf{x}'$ will be denoted by a prime. Substitution of the old variables by the rescaled ones in the free energy (5) leads to

$$\Delta F=\frac{1}{V'}\int d^3x'\left[\alpha|\Delta_\lambda(\mathbf{x}')|^2+\frac{\beta}{2}|\Delta_\lambda(\mathbf{x}')|^4+\frac{1}{\lambda^2}\frac{1}{2m^*}\left|\left(\frac{\hbar}{i}\nabla'-\frac{2e}{c}\mathbf{A}_\lambda\right)\Delta_\lambda(\mathbf{x}')\right|^2+\frac{1}{\lambda^4}\frac{1}{8\pi}[\mathrm{curl}'\mathbf{A}_\lambda(\mathbf{x}')]^2\right], \tag{14}$$

and changes the boundary conditions to

$$\mathbf{A}_\lambda(\mathbf{x}'+\mathbf{b}'_\nu)=\mathbf{A}_\lambda(\mathbf{x}')+\nabla'\chi_{\lambda\nu}(\mathbf{x}')\,, \tag{15}$$

$$\Delta_\lambda(\mathbf{x}'+\mathbf{b}'_\nu)=\Delta_\lambda(\mathbf{x}')\exp\left[i\frac{2e}{\hbar c}\chi_{\lambda\nu}(\mathbf{x}')\right]. \tag{16}$$

The quantum numbers $N_{\alpha\beta}$ are unchanged, but Eq. (10) implies a changed average magnetic field,

$$\mathbf{B}_\lambda\equiv\tfrac{1}{2}N_{\alpha\beta}\epsilon_{\alpha\beta\gamma}\mathbf{b}'_\gamma\Phi_0/V'=\lambda^2\mathbf{B}\,. \tag{17}$$

Thus we have shown the following scaling property of the Ginzburg-Landau free energy: The *constrained minimum* of the free energy is *unchanged* when the kinetic energy term is multiplied by a factor $1/\lambda^2$, the field energy term by a factor $1/\lambda^4$, and the average field by a factor λ^2.

We next differentiate the free energy with respect to λ, set $\lambda=1$, and obtain from $\partial\Delta F/\partial\lambda=0$,

$$0=-2F_{\mathrm{kin}}-4F_{\mathrm{field}}+\frac{\partial\Delta F}{\partial\mathbf{B}}\cdot 2\mathbf{B}\,. \tag{18}$$

In calculating $\partial\Delta F/\partial\lambda$ we can neglect the λ dependence of Δ and $\mathbf{A}$ because of the stationarity of ΔF under variations of Δ and $\mathbf{A}$. Equation (18) and the thermodynamic relation (6) together give us directly the virial theorem in the special case that $F_{\mathrm{inhom}}=0$.

In the generalized virial theorem (1), the additional term F_{inhom} arises if the material parameters α, β, and m^* of the Ginzburg-Landau theory depend on $\mathbf{x}$. In this case, a change of the length scale also affects the "constants" α,

β, and m^*, and leads to additional λ dependences in Eq. (14) that require one to replace α, β, and m^* by

$$\alpha_\lambda(\mathbf{x}')\equiv\alpha(\lambda\mathbf{x}'),\quad \beta_\lambda(\mathbf{x}')\equiv\beta(\lambda\mathbf{x}'),\quad m_\lambda^*(\mathbf{x}')\equiv m^*(\lambda\mathbf{x}') .$$

Consequently, the derivative $\partial\Delta F/\partial\lambda$ at $\lambda=1$ has an additional term which we denote by F_{inhom}:

$$F_{\text{inhom}}=\frac{1}{V}\int d^3x\left[[\mathbf{x}\cdot\nabla\alpha(\mathbf{x})]\,|\Delta(\mathbf{x})|^2+\tfrac{1}{2}[\mathbf{x}\cdot\nabla\beta(\mathbf{x})]\,|\Delta(\mathbf{x})|^4-[\mathbf{x}\cdot\nabla m^*(\mathbf{x})]\frac{1}{2m^*(\mathbf{x})^2}\left|\left(\frac{\hbar}{i}\nabla-\frac{2e}{\hbar c}\mathbf{A}\right)\Delta(\mathbf{x})\right|^2\right] . \tag{19}$$

F_{inhom} adds on to the right-hand side of Eq. (18), which leads to the generalized virial theorem (1).

III. CONCLUSION

It is straightforward to derive a more generalized virial theorem which holds for each single component of **B** and **H**. One simply has to scale the three space directions by different factors. The less general version (1), however, is sufficient for most purposes, in particular, if the directions of the magnetic fields are known from symmetry considerations. It is also straightforward to generalize the virial theorem to anisotropic superconductors and to temperatures outside the Ginzburg-Landau range.

An obvious application of the theorem is the evaluation of the applied field **H** for a given averaged total field. The most costly part of such a calculation is the determination of the equilibrium magnetic field $\mathbf{B}(\mathbf{x})$ and order parameter $\Delta(\mathbf{x})$ at fixed average field, either by solving the Ginzburg-Landau equations or by other means. The standard calculation of the external field from Eq. (6) requires doing the costly part at least 2 times in order to numerically get the derivative of the free energy with respect to the average field. Formula (1), on the other hand, requires nearly no additional calculations, since all the needed quantities are already available from a single determination of the equilibrium field and order parameter, and allows one to avoid the often error inducing process of numerical differentiation.

The Ginzburg-Landau equations have been extensively studied, and the virial theorem (1) can easily be derived by common arguments. Hence, it is possible that this theorem can be found somewhere in the literature, although we do not know where.

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