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Energy of a Lattice of Quantized Flux Lines*

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Analytic expressions are given for the magnetic flux density B and the Gibbs free energy G of a bulk type-II superconductor in an intermediate magnetic field H_0 ($H_{c1} \ll H_0 \ll H_{c2}$). Both square and triangular lattices are considered; the triangular lattice is confirmed as the more stable structure.

I. INTRODUCTION

In the mixed state of bulk type-II superconductors, the magnetic field penetrates the sample in the form of quantized flux lines.[1] Each line consists of a core surrounded by circulating supercurrent. The radius of the core is given approximately by the coherence length ξ. Outside of the core, the magnitude of the circulating supercurrent decreases inversely with the radius r out to the penetration depth λ, beyond which the supercurrent vanishes exponentially. The present work is restricted to extreme type-II behavior, which is characterized by a large value of the ratio $\kappa = \lambda/\xi$; in this limit, the core of the flux line may be treated as a singularity in the current distribution, and the structure of the line is similar to that of a classical vortex filament.

The theory of the mixed state takes a different form in each of three distinct regions of magnetic field strength H_0,[1] corresponding to different values of the density of flux lines. In the low-density region ($H_0 \gtrsim H_{c1}$, where H_{c1} is the lower critical field), the distance d between the lines is much greater than the penetration depth λ, so that the lines may be considered independently. In the intermediate-density region ($H_{c1} \ll H_0 \ll H_{c2}$, where H_{c2} is the upper critical field), the separation lies in the interval $\xi \ll d \ll \lambda$, and the lines interact appreciably. Finally for $H_0 \lesssim H_{c2}$, the separation of the lines is comparable with the core radius ξ, and the precise structure of the core becomes important.

It is generally assumed[1–3] that the stable configuration in the intermediate-density regime is a regular two-dimensional lattice. The properties of the bulk sample are thus expressed in terms of well-defined lattice sums, which have previously been obtained only through computer calculations.[2] A mathematical technique for the evaluation of such sums has been developed[3] in a form that converges rapidly for $\xi \ll d \ll \lambda$. Here, these analytic summation formulas are applied to the calculation of the magnetic flux density B and the Gibbs free energy G of square and triangular lattices as a function of the applied magnetic field in the region of intermediate density.

In Sec. II, we review briefly the properties of bulk type-II superconductors, introducing the necessary lattice sums for both square and triangular lattices. The physically interesting quantities B and G are evaluated in Sec. III.

II. BULK TYPE-II SUPERCONDUCTORS

In a type-II superconductor, the singular behavior of the circulating supercurrent near each flux line requires a modification of London's phenomenological theory of superconductivity.[4] The extended London equation is[5]

$$\nabla \times \mathbf{j} + (c/4\pi\lambda^2)\mathbf{H} = (\varphi_0 c/4\pi\lambda^2)\hat{z} \sum_j \delta(\mathbf{r}-\mathbf{r}_j), \tag{1}$$

where the summation runs over all the flux lines in the sample. The magnetic field $\mathbf{H}$ is parallel to $\hat{z}$ (a unit vector along the z axis) and $\varphi_0 = (2\pi\hbar c/2e)$ is the quantum of magnetic flux. The vector $\mathbf{r}$ lies in the xy plane, so that $\delta(\mathbf{r})$ is a two-dimensional delta function.

From Eq. (1) and Maxwell's equation $\nabla \times \mathbf{H} = (4\pi/c)\,\mathbf{j}$ it is not difficult to derive the interaction energy V_{12} of two vortices at $\mathbf{r}_1$ and $\mathbf{r}_2$[1–3]:

$$V_{12} = (\varphi_0^2/8\pi^2\lambda^2)K_0(r_{12}/\lambda), \tag{2}$$

where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$, and K_0 is the Bessel function that vanishes exponentially for large values of its argument.[6] The total interaction energy V per unit length of the lattice is

$$V = \tfrac{1}{2} \sum_{ij}{}' V_{ij}, \tag{3}$$

where the summation is over i and j separately, omitting the terms $i = j$. Since V_{ij} depends only on the distance between $\mathbf{r}_i$ and $\mathbf{r}_j$, Eq. (3) can be rewritten as

$$V = \tfrac{1}{2} N \sum_j{}' V_{0j}, \tag{4}$$

where N is the number of flux lines in the sample. The total free energy per unit volume F is

$$F = n\epsilon_1 + (n\varphi_0^2/16\pi^2\lambda^2) \sum_j{}' K_0(r_{0j}/\lambda). \tag{5}$$

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[1] A. A. Abrikosov, Zh. Eksperim. i Teor. Fiz. **32**, 1442 (1957) [English transl.: Soviet Phys.—JETP **5**, 1174 (1957)].

[2] P. G. de Gennes and J. Matricon, Rev. Mod. Phys. **36**, 45 (1964); J. Matricon, Phys. Letters **9**, 289 (1964).

[3] A. L. Fetter, P. C. Hohenberg, and P. Pincus, preceding paper, Phys. Rev. **147**, 140 (1966).

[4] F. London, *Superfluids* (Dover Publications, Inc., New York, 1961), Vol. I, Sec. B.

[5] See, for example, A. A. Abrikosov, M. P. Kemoklidze, and I. M. Khalatnikov, Zh. Eksperim. i Teor. Fiz. **48**, 765 (1965) [English transl.: Soviet Phys.—JETP **21**, 506 (1965)].

[6] We follow the notation of G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, Cambridge, England, 1962), 2nd ed., Chap. III.

Here ϵ_1 is the energy per unit length of a single flux line, and n is the number of lines per unit area.

The equilibrium magnetic flux density $B=n\varphi_0$ is obtained by minimizing the Gibbs free energy (thermodynamic potential) G per unit volume with respect to B,[1,2] where G is related to F by a Legendre transformation[7]

$$G=F-(4\pi)^{-1}BH_0. \tag{6}$$

Equation (6) depends on B both explicitly and indirectly since r_{0j} is proportional to $B^{-1/2}$. The condition $dG/dB=0$ yields the following implicit equation for the magnetic flux density B as a function of the applied field H_0:

$$H_0=H_{c1}+(\varphi_0/8\pi\lambda^2)\sum_j{}'\{2K_0(r_{0j}/\lambda)+\tfrac{1}{2}(r_{0j}/\lambda)^2[K_2(r_{0j}/\lambda)-K_0(r_{0j}/\lambda)]\}, \tag{7}$$

where $H_{c1}=4\pi\epsilon_1/\varphi_0$. The Gibbs free energy, which is a function of H_0, is then obtained from Eqs. (6) and (7),

$$G=-(B\varphi_0/64\pi^2\lambda^4)\sum_j{}' r_{0j}{}^2[K_2(r_{0j}/\lambda)-K_0(r_{0j}/\lambda)]. \tag{8}$$

The following theorem[8] has been used in the derivation of both Eqs. (7) and (8):

$$dK_0(x)/dx=-K_1(x)=\tfrac{1}{2}x[K_0(x)-K_2(x)]. \tag{9}$$

Equations (7) and (8) express the magnetic flux density and Gibbs free energy in terms of certain sums over all lattice sites (excluding the origin). It is convenient to introduce a simplified notation.

$$\Sigma_0=\sum_j{}' K_0(r_{0j}/\lambda), \tag{10a}$$

$$\Sigma_1=d^{-2}\sum_j{}' r_{0j}{}^2K_0(r_{0j}/\lambda), \tag{10b}$$

$$\Sigma_2=d^{-2}\sum_j{}' r_{0j}{}^2K_2(r_{0j}/\lambda). \tag{10c}$$

When the distinction between square and triangular lattices becomes important, Eq. (10) will be written with an additional subscript 4 or 6 (for the four fold or six fold rotational symmetry). In terms of these sums, Eqs. (7) and (8) may be rewritten as

$$H_0=H_{c1}+(\varphi_0/8\pi\lambda^2)[2\Sigma_0+\tfrac{1}{2}\mu^2(\Sigma_2-\Sigma_1)], \tag{11}$$

$$G=-(B\varphi_0/64\pi^2\lambda^2)\mu^2(\Sigma_2-\Sigma_1), \tag{12}$$

where $\mu=d/\lambda$.

The sum Σ_0 may be easily obtained from the results of Ref. 3, where Σ_1 and Σ_2 have been evaluated explicitly. We find, for the square and triangular lattices, respectively,

$$\begin{aligned}\Sigma_{04}&=(2\pi/\mu^2)+\tfrac{1}{2}\ln\mu^2-\tfrac{1}{2}[\ln(4\pi)+1-\gamma]+\tfrac{1}{2}A_4+O(\mu^2),\\ \Sigma_{14}&=(8\pi/\mu^4)+O(1),\\ \Sigma_{24}&=(16\pi/\mu^4)-(2/\mu^2)+O(\mu^2);\end{aligned} \tag{13}$$

$$\begin{aligned}\Sigma_{06}&=(4\pi/\sqrt{3}\mu^2)+\tfrac{1}{2}\ln\mu^2-\tfrac{1}{2}[\ln(8\pi/\sqrt{3})+1-\gamma]+\tfrac{1}{2}A_6+O(\mu^2),\\ \Sigma_{16}&=(16\pi/\sqrt{3}\mu^4)+O(1),\\ \Sigma_{26}&=(32\pi/\sqrt{3}\mu^4)-(2/\mu^2)+O(\mu^2).\end{aligned} \tag{14}$$

Here $\gamma(=0.5772\cdots)$ is Euler's constant, and the constants A_4 and A_6 are given by

$$A_4=\sum_{lm}{}'\{E_1[\pi(l^2+m^2)]+\pi^{-1}(l^2+m^2)^{-1}\times\exp[-\pi(l^2+m^2)]\}\approx 0.10087, \tag{15a}$$

$$A_6=\sum_{lm}{}'\{E_1[(2\pi/\sqrt{3})(l^2+lm+m^2)]+[(2\pi/\sqrt{3})\times(l^2+lm+m^2)]^{-1}\exp[-(2\pi/\sqrt{3})(l^2+lm+m^2)]\}\approx 0.07968. \tag{15b}$$

The exponential integral in Eq. (15) is defined as[9]

$$E_1(x)=\int_x^\infty dt\, t^{-1}e^{-t}. \tag{16}$$

The series converges very rapidly, so that the third-nearest neighbors are sufficient to obtain an accuracy of five significant figures.

III. PHYSICAL PROPERTIES OF THE LATTICE

The Gibbs free energy has been expressed [Eq. (12)] in terms of the lattice sums. Substitution of Eqs. (13) and (14) yields for the square and triangular lattices, respectively,

$$G_4=-(B_4\varphi_0/64\pi^2\lambda^2)[(8\pi/\mu^2)-2+O(\mu^2)], \tag{17a}$$

$$G_6=-(B_6\varphi_0/64\pi^2\lambda^2)[(16\pi/\sqrt{3}\mu^2)-2+O(\mu^2)]. \tag{17b}$$

The density of lines n is given by $n=d^{-2}$ for the square lattice and $n=(2/\sqrt{3})d^{-2}$ for the triangular lattice; the magnetic flux density B is equal to $n\varphi_0$ in both lattices. Equations (17a) and (17b) become identical when expressed in terms of the magnetic flux density,

$$G_4=-B_4{}^2/8\pi+B_4\varphi_0/32\pi^2\lambda^2+O(1), \tag{18a}$$

$$G_6=-B_6{}^2/8\pi+B_6\varphi_0/32\pi^2\lambda^2+O(1). \tag{18b}$$

The difference between the Gibbs free energy of the two lattices is due entirely to the difference in the magnetic flux density for the same applied magnetic field. The relation between B and H_0 has been given in Eq. (11). For the square and triangular lattices,

$$\begin{aligned}H_0-H_{c1}&=(\varphi_0/8\pi\lambda^2)[(8\pi/\mu^2)+\ln\mu^2-\ln(4\pi)-2+\gamma+A_4]+O(\mu^2)\\ &=B_4+(\varphi_0/8\pi\lambda^2)[\ln(\varphi_0/B_4\lambda^2)-\ln(4\pi)-2+\gamma+A_4]+O(B_4{}^{-1}),\end{aligned} \tag{19a}$$

[7] Reference 4, p. 18.

[8] H. B. Dwight, *Tables of Integrals and Other Mathematical Data* (The Macmillan Company, New York, 1957), 3rd ed., p. 177.

[9] We follow the notation of *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, edited by M. Abramowitz and I. A. Stegun (U. S. Government Printing Office, Washington, D. C., 1964), Natl. Bur. Std. Appl. Math. Ser. 55, p. 228.

$$
\begin{aligned}
H_0-H_{c1}&=(\varphi_0/8\pi\lambda^2)[(16\pi/\sqrt{3}\mu^2)+\ln\mu^2-\ln(8\pi/\sqrt{3})\\
&\qquad-2+\gamma+A_6]+O(\mu^2)\\
&=B_6+(\varphi_0/8\pi\lambda^2)[\ln(\varphi_0/B_6\lambda^2)-\ln(4\pi)\\
&\qquad-2+\gamma+A_6]+O(B_6^{-1})\,.
\end{aligned}\tag{19b}
$$

These equations may be inverted to first order

$$
\begin{aligned}
B_4\approx H_0-H_{c1}+(\varphi_0/8\pi\lambda^2)\{&\ln[\lambda^2(H_0-H_{c1})/\varphi_0]\\
&+\ln(4\pi)+2-\gamma-A_4\}\,,
\end{aligned}\tag{20a}
$$

$$
\begin{aligned}
B_6\approx H_0-H_{c1}+(\varphi_0/8\pi\lambda^2)\{&\ln[\lambda^2(H_0-\mathrm{H}_{c1})/\varphi_0]\\
&+\ln(4\pi)+2-\gamma-A_6\}\,,
\end{aligned}\tag{20b}
$$

neglecting terms of order

$$(\varphi_0/\lambda^2)^2(H_0-H_{c1})^{-1}\ln[\lambda^2(H_0-H_{c1})/\varphi_0]\,.$$

For a given magnetic field, the magnetic flux density in the two lattices differs only by the constant A that depends on the detailed lattice structure.

The Gibbs free energy can now be computed from Eqs. (18) and (20):

$$
\begin{aligned}
G_4=-(8\pi)^{-1}(H_0-H_{c1})^2-(32\pi^2\lambda^2)^{-1}(H_0-H_{c1})\varphi_0&\\
\times\{\ln[\lambda^2(H_0-H_{c1})/\varphi_0]&\\
+\ln(4\pi)+1-\gamma-A_4\}\,,&
\end{aligned}\tag{21a}
$$

$$
\begin{aligned}
G_6=-(8\pi)^{-1}(H_0-H_{c1})^2-(32\pi^2\lambda^2)^{-1}(H_0-H_{c1})\varphi_0&\\
\times\{\ln[\lambda^2(H_0-H_{c1})/\varphi_0]&\\
+\ln(4\pi)+1-\gamma-A_6\}\,.&
\end{aligned}\tag{21b}
$$

The difference in the Gibbs free energy is

$$
\begin{aligned}
G_4-G_6&=(32\pi^2\lambda^2)^{-1}(H_0-H_{c1})\varphi_0(A_4-A_6)\\
&\approx(32\pi^2\lambda^2)^{-1}(H_0-H_{c1})\varphi_0(0.02119)\,.
\end{aligned}\tag{22}
$$

The triangular lattice has a lower Gibbs free energy and represents the more stable configuration.[1,2] Small corrections to Eq. (22) arise from the terms neglected in Eq. (19) and are independent of H_0-H_{c1}.

The present approach cannot preclude a *metastable* square lattice structure; a detailed calculation[2,3] shows, however, that the square lattice is dynamically unstable with respect to small perturbations of the flux lines from their equilibrium position, while the triangular lattice is dynamically stable. The triangular lattice has also been shown to have the lower Gibbs free energy in both the low-density region[1] ($H_{c1}\lesssim H_0$) and the high-density region[10] ($H_0\lesssim H_{c2}$), so that this structure is expected to occur for all values of applied magnetic field.

The same sums may be used to calculate the contribution to the specific heat of a type-II superconductor due to the lattice of flux lines.[11] Similar techniques may also prove useful in the study of thin superconducting films in perpendicular magnetic fields, where a related lattice structure occurs.[12]

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