$$F(a)=\frac{1}{2}\int_0^\infty \frac{t^{-3/4}e^{-t/2}M_{-1/4,1/4}(t)}{a^2+t}$$

$$=\tfrac{1}{4}a^{-3/2}G^{22}_{23}\left(a^2\,\middle|\,{}^{3/4\;5/4}_{3/4\;3/4\;1/4}\right),$$

which is a known Stieltjes transform.[8]

APPENDIX B

Let

$$I_1=2\int_0^1 dz\,J_0[x(1-z)^{1/2}]\begin{cases}\cos(px^2z^2)\\ \sin(px^2z^2)\end{cases}.$$

We note the Fourier cosine transform pairs

$$\eta_+(1-z)J_0[x(1-z^2)^{1/2}]\bullet\!\sim\!\circ\,(x^2+y^2)^{-1/2}\sin(x^2+y^2)^{1/2},$$

$$\begin{matrix}\cos(px^2z^2)\\ \sin(px^2z^2)\end{matrix}\Big\}\bullet\!\sim\!\bullet\,\frac{1}{4x}\left(\frac{2\pi}{p}\right)^{1/2}\left[\cos\left(\frac{y^2}{4px^2}\right)\pm\sin\left(\frac{y^2}{4px^2}\right)\right].$$

So, by Parseval's theorem, we have

$$I_1=\frac{1}{x}\left(\frac{2}{\pi p}\right)^{1/2}\int_0^\infty(1+y^2)^{-1/2}\sin[x(1+y^2)^{1/2}]\times\left[\cos\left(\frac{y^2}{4p}\right)\pm\sin\left(\frac{y^2}{4p}\right)\right]dy.$$

Next, note that

$$I_2=\int_0^\infty dx\,x^{-3/2}J_{3/2}(x)\sin(ax)$$

$$=(\tfrac{1}{2}\pi a)^{1/2}\int_0^\infty dx\,x^{-1}J_{3/2}(x)J_{1/2}(ax),$$

where

$$a=(1+y^2)^{1/2},$$

which is a Weber-Schaftheitlin integral and has the value

$$I_2=\tfrac{1}{3}a^{-1}(2/\pi)^{1/2}\,{}_2F_1(\tfrac{1}{2},1;\tfrac{5}{2};1/a^2)$$

$$=\frac{1}{4}\left(\frac{2}{\pi}\right)^{1/2}(1-a^2)\left[\ln\left(\frac{a+1}{a-1}\right)+\frac{2a}{1-a^2}\right],\quad a>1.$$

Thus we obtain

$$\begin{matrix}C(p)\\ S(p)\end{matrix}\Big\}=\left(\frac{1}{2\pi}\right)p^{-1/2}\int_0^\infty dy\,y^2(1+y^2)^{-1/2}\times\left[2y^{-2}(1+y^2)^{1/2}+\ln\left(\frac{(1+y^2)^{1/2}-1}{(1+y^2)^{1/2}+1}\right)\right]\times\left[\cos\left(\frac{y^2}{4p}\right)\pm\sin\left(\frac{4^2}{4p}\right)\right],$$

which is equivalent to (3.6) and (3.7).

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Magnetization of Dirty Superconductors near the Upper Critical Field*

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The magnetic behavior of a type-II superconductor with very short electron mean free path (dirty limit) near its upper critical field $B_{c2}(T)$ is investigated. A calculation of the magnetization up to the second order in the difference between $B_{c2}(T)$ and the external magnetic field is presented which is valid for all temperatures. A triangular and a square lattice of flux lines are considered. A numerical calculation suggests that the triangular lattice remains stable despite the fact that the difference in the thermodynamical potentials between the two lattices decreases due to these second-order terms.

I. INTRODUCTION

The magnetic behavior of type-II superconductors was first explained theoretically by Abrikosov.[1] On the basis of the Ginzburg-Landau theory,[2] Abrikosov showed that a type-II superconductor exhibits a mixed state between the two critical magnetic fields $B_{c1}(T)$ and $B_{c2}(T)$ in which the magnetic flux penetrates the specimen in the form of quantized flux lines. The Ginzburg-Landau equations were shown by Gorkov[3] to follow from the microscopic theory of superconductivity near the transition temperature T_c of the metal in zero magnetic field, and only there. Many attempts have therefore been made to generalize Abrikosov's work to lower temperatures.[4] Recently, the vicinity of the upper critical field $B_{c2}(T)$ was treated completely by Eilenberger[5] who calculated the parameters $\kappa_1(T)$ and $\kappa_2(T)$ numerically for all temperatures and all electron mean free paths. These parameters are directly related to the upper critical field $B_{c2}(T)$ and to the slope of the magnetization at $B_{c2}(T)$, respectively. The behavior in the vicinity of the lower critical field $B_{c1}(T)$ is known only near T_c and for materials with high κ values.[4] To the author's knowledge very little is known about a generalization of Abrikosov's theory to fields well below B_{c2}.

The present paper deals with the magnetization of a type-II superconductor near its upper critical field B_{c2}. Starting from a generalized diffusion equation derived earlier by the author[6] the magnetization is calculated up to the second order in the quantity $(B_e - B_{c2})$, where B_e denotes the external magnetic field. The calculation is restricted to dirty superconductors—where our diffusion equation is valid—within the framework of the weak-coupling theory of superconductivity. But our theory is valid for all temperatures.

The slope of the magnetization at B_{c2} for dirty superconductors and for all temperatures was first calculated by Maki[7] and later on corrected by Caroli *et al.*[8] This corrected version of Caroli *et al.* was confirmed by Eilenberger's[5] numerical calculations. Our results for the slope of the magnetization agree with these findings. The most interesting aspect of these calculations is the fact that the triangular arrangement of flux lines gives the thermodynamically stable configuration as opposed to the square lattice. This statement is even true for all temperatures and all electron mean free paths, as was shown by Eilenberger.[5] But the difference in the thermodynamical potentials between these two lattices is rather small. Therefore, it is an interesting question whether the above statement remains true if one takes higher-order terms of the quantity $(B_e - B_{c2})$ into account. Our calculations show that the second term in this expansion in fact has the tendency to reduce this difference. This reduction, however, seems not to be strong enough to lead to a transition from a triangular lattice, established near B_{c2}, to a square lattice at lower fields, and it certainly is not strong enough for such a transition at temperatures near T_c. Furthermore we find that the second-order term generally is very small, suggesting that the magnetization remains very linear for fields B_e well below B_{c2}. This finding agrees very well with magnetization measurements.

II. PROPERTIES OF EXACT SOLUTIONS

A superconductor with very short electron mean free path can be described by the following set of equations derived earlier by the author[6]:

$$\omega F_\omega(\vec{r}) - \tfrac{1}{2}D[G_\omega(\vec{r})\vec{\partial}^2 F_\omega(\vec{r}) - F_\omega(\vec{r})\vec{\partial}^2 G_\omega(\vec{r})] = \Delta(\vec{r})G_\omega(\vec{r}) \,, \quad (1)$$

$$G_\omega(\vec{r}) = (1 - |F_\omega(\vec{r})|^2)^{1/2} \,, \quad (2)$$

$$\Delta(\vec{r})\ln\left(\frac{T}{T_c}\right) = 2\pi T \sum_{\omega>0}\left(F_\omega(\vec{r}) - \frac{\Delta(\vec{r})}{\omega}\right) \,, \quad (3)$$

$$\vec{j}(\vec{r}) = \frac{1}{4\pi}\,\mathrm{curl}\,\mathrm{curl}(\vec{B}(\vec{r}) - \vec{B}_e(\vec{r})) = 2ieN(0)D\pi T \sum_{\omega>0}[F_\omega^*(\vec{r})\vec{\partial}F_\omega(\vec{r}) - \text{c. c.}] \,. \quad (4)$$

Equation (1) follows easily from Eq. (11) of Ref. 6 if Eq. (2) is used. The notation is the same as that introduced in Ref. 6.

We are looking for solutions of the above set of equations which show the structure of the vortex-line lattice introduced by Abrikosov.[1] We therefore assume that the internal magnetic field $\vec{B}(\vec{r})$ is a periodic function in the x-y plane, say, $\vec{B}(\vec{r}) = B(x, y)\hat{z}$. The external magnetic field B_e is assumed to be constant in space. Clearly it has to be parallel to $\vec{B}(\vec{r})$, $\vec{B}_e = B_e\hat{z}$. Furthermore we assume that both $\Delta(\vec{r})$ and $F_\omega(\vec{r})$ depend only on x and y and that $|\Delta(\vec{r})|$ and $|F_\omega(\vec{r})|$ are periodic in the same manner as $B(x, y)$.

The first important conclusion then follows from Eq. (4). Let us denote the unit-cell vectors of the flux-line lattice by $\vec{e}_j = (x_j, y_j, 0)$, $j = 1, 2$. Since $\vec{B}(\vec{r})$ is a periodic function and since $\vec{A}(\vec{r})$ is defined by

$$\mathrm{curl}(\vec{A}(\vec{r})) = \vec{B}(\vec{r}), \quad (5)$$

the relations

$$\vec{A}(\vec{r} + \vec{e}_j) = \vec{A}(\vec{r}) + \vec{\partial}\chi(\vec{r}, \vec{e}_j), \quad j = 1, 2 \quad (6)$$

must hold true with certain functions $\chi(\vec{r}, \vec{e}_j)$. It follows then from Eq. (4), i.e., from the periodicity of the current density, that $F_\omega(\vec{r})$ behaves like

$$F_\omega(\vec{r} + \vec{e}_j) = F_\omega(\vec{r})\exp\{-2ie[\chi(\vec{r}, \vec{e}_j) + K(\vec{e}_j)]\}, \quad (7)$$

and $K(\vec{e}_j)$ are constants. From Eqs. (1) and (3) the same behavior for the pair potential $\Delta(\vec{r})$ follows:

$$\Delta(\vec{r} + \vec{e}_j) = \Delta(\vec{r})\exp\{-2ie[\chi(\vec{r}, \vec{e}_j) + K(\vec{e}_j)]\} \,. \quad (8)$$

Equations (6) and (8) together with the requirement that $\Delta(r)$ is a single-valued function lead already to the flux quantization. This is well known from the Ginzberg-Landau theory. We will assume from the very beginning that the flux through a unit cell of the lattice is given by one flux quantum,

$$\bar{B}\mathfrak{F} = \pi/e \ , \tag{9}$$

where $\mathfrak{F}$ denotes the area of a cell and $\bar{B}$ the averaged magnetic field

$$\bar{B} = (1/\mathfrak{F}) \int_{\text{cell}} dx\, dy\, B(x,y) \equiv \langle B(\vec{r}) \rangle . \tag{10}$$

Without any loss of generality we now write

$$\vec{e}_1 = (x_1, 0, 0), \quad \vec{e}_2 = (x_2, y_2, 0), \tag{11}$$

and

$$\vec{A}(\vec{r}) = -\bar{B}y\hat{x} + \vec{A}'(\vec{r}), \tag{12}$$

with

$$\vec{A}'(\vec{r}+\vec{e}_i) = \vec{A}'(\vec{r}), \quad \bar{\vec{B}}' = \langle \text{curl}(\vec{A}'(\vec{r})) \rangle = 0 . \tag{13}$$

It is then an easy matter to show that one can replace Eqs. (7) and (8) without loss of generality by

$$\begin{aligned} &F_\omega(\vec{r}+\vec{e}_1) = F_\omega(\vec{r}), \quad \Delta(\vec{r}+\vec{e}_1) = \Delta(\vec{r}), \\ &F_\omega(\vec{r}+\vec{e}_2) = \exp[2ie\bar{B}y_2(x+x_2/2)]\, F_\omega(\vec{r}), \\ &\Delta(\vec{r}+\vec{e}_2) = \exp[2ie\bar{B}y_2(x+x_2/2)]\, \Delta(\vec{r}). \end{aligned} \tag{14}$$

All the above statements are simply generalizations of relations known from Ginzburg-Landau theory. The reader who is interested in more details is referred to Ref. 9.

III. SERIES EXPANSIONS OF BASIC EQUATIONS

We are interested in solutions of Eqs. (1)-(4) near the upper critical field B_{c2}. In this region a small parameter is given by the difference $B_{c2} - \bar{B}$ since $\bar{B}$ approaches B_{c2} continuously as the transition curve is reached. In Eqs. (1)-(4) an expansion of all relevant quantities into powers of $B_{c2} - \bar{B}$ should therefore be possible. But in order to use the exact relations derived in Sec. II it is very essential to keep $\bar{B}$ fixed during this expansion. This means that in the following we will consider B_{c2} as an adjustable quantity. B_{c2} is given as a function of temperature T and transition temperature T_c by the well-known expression

$$\ln\left(\frac{T}{T_c}\right) = 2\pi T \sum_{\omega>0}\left(\frac{1}{\omega + DeB_{c2}(T, T_c)} - \frac{1}{\omega}\right). \tag{15}$$

It is now very convenient to keep not only $\bar{B}$ but also T fixed so that B_{c2} is now considered to vary only due to variations of T_c. The reason for this is that the only equation which contains T_c explicitly is the self-consistency relation (3); Eqs. (1), (2), and (4) depend only on quantities now considered as fixed, i.e., $\bar{B}$ and T. Let us then define the parameters

$$\rho_c = DeB_{c2}(T, T_c), \quad \rho = De\bar{B}. \tag{16}$$

The relation between T_c and the expansion parameter

$$\lambda = \rho_c - \rho \tag{17}$$

then follows immediately from Eq. (15),

$$\ln\left(\frac{T}{T_c}\right) = 2\pi T \sum_{\omega>0}\left(\frac{1}{\omega+\rho+\lambda} - \frac{1}{\omega}\right) . \tag{18}$$

This equation expresses λ as a function of T_c and vice versa. For small λ we can expand

$$\ln\left(\frac{T}{T_c}\right) = l_0 + l_1\lambda + l_2\lambda^2 + \cdots , \tag{19}$$

with

$$\begin{aligned} l_0 &= 2\pi T \sum_{\omega>0}\left(\frac{1}{\omega+\rho} - \frac{1}{\omega}\right), \\ l_1 &= -2\pi T \sum_{\omega>0} \frac{1}{(\omega+\rho)^2}, \ \ldots . \end{aligned} \tag{20}$$

Next we expand the quantities Δ, F_ω, and $\vec{A}'$ into powers of λ. Inspection of Eqs. (1)-(4) shows immediately that these power series must have the structure

$$\begin{aligned} \Delta &= (\surd\lambda)(\Delta_0 + \lambda\Delta_1 + \lambda^2\Delta_2 + \cdots), \\ F &= (\surd\lambda)(F_0 + \lambda F_1 + \lambda^2 F_2 + \cdots), \\ G &= 1 + \lambda G_1 + \lambda^2 G_2 + \cdots , \\ \vec{A}' &= \lambda\vec{a}_1 + \lambda^2\vec{a}_2 + \cdots . \end{aligned} \tag{21}$$

Here we have dropped the arguments $\vec{r}$ and ω. The quantities Δ_ν, F_ν, and a_ν depend only on $\bar{B}$ and T. They are assumed to fulfill the boundary conditions (13) and (14).

We would like to make some further remarks on the above series. First of all we cannot prove whether the above series are convergent. But nevertheless we believe that it makes sense to consider the first few terms in these expansions. Disregarding this difficulty we see that the above method gives solutions of the basic equations for a fixed averaged magnetic field $\bar{B}$ and for fixed unit cell of the fluxoid lattice. The actual magnetic field $\bar{B}$ as a function of the external parameters B_e and T, as well as the shape of the fundamental cell, have to be determined by minimizing the thermodynamical potential. This will be formulated in Sec. IV.

Let us now write the first few equations which follow from Eqs. (1) to (4) by inserting the series (19) and (21). We continue to drop the obvious arguments $\vec{r}$, ω. From Eqs. (2) and (21) it follows that

$$G_1 = -\tfrac{1}{2}|F_0|^2, \tag{22}$$

$$G_2 = -\tfrac{1}{8}|F_0|^4 - \tfrac{1}{2}(F_0F_1^* + \text{c.c.}). \quad (23)$$

We define the symbol

$$\vec{\tilde{\partial}}_0 = \vec{\partial} - 2ie\bar{B}y\hat{x}. \quad (24)$$

From Eqs. (1), (21), and (22) it then follows that

$$\omega F_0 - \tfrac{1}{2}D\vec{\tilde{\partial}}_0^2 F_0 = \Delta_0, \quad (25)$$

$$\omega F_1 - \tfrac{1}{2}D\vec{\tilde{\partial}}_0^2 F_1 = R_1 + \Delta_1, \quad (26)$$

with R_1 given by

$$R_1 = -\tfrac{1}{2}\Delta_0|F_0|^2 + \tfrac{1}{2}D[-\tfrac{1}{2}|F_0|^2\vec{\tilde{\partial}}_0^2F_0 + 2ie(\vec{\tilde{\partial}}_0\cdot\vec{a}_1 + \vec{a}_1\cdot\vec{\tilde{\partial}}_0)F_0 + \tfrac{1}{2}F_0\vec{\partial}^2|F_0|^2] \quad (27)$$

and

$$\omega F_2 - \tfrac{1}{2}D\vec{\tilde{\partial}}_0^2 F_2 = R_2 + \Delta_2. \quad (28)$$

R_2 is a fairly long expression and we will not write it here. From Eqs. (4) and (21) it follows that

$$\vec{j}_1 = \frac{1}{4\pi}\,\text{curl}\,\text{curl}\,\vec{a}_1 = 2ieDN(0)\pi T\sum_{\omega>0}(F_0^*\vec{\tilde{\partial}}_0F_0 - \text{c.c.}), \quad (29)$$

$$\vec{j}_2 = \frac{1}{4\pi}\,\text{curl}\,\text{curl}\,\vec{a}_2 = 2ieDN(0)\pi T\sum_{\omega>0}[(F_0^*\vec{\tilde{\partial}}F_1 + F_1^*\vec{\tilde{\partial}}_0F_0) - \text{c.c.} + 4ie\,\vec{a}_1|F_0|^2]. \quad (30)$$

Finally we get from Eqs. (3), (19), and (21)

$$\Delta_0 l_0 = 2\pi T\sum_{\omega>0}\left(F_0 - \frac{\Delta_0}{\omega}\right), \quad (31)$$

$$\Delta_0 l_1 + \Delta_1 l_0 = 2\pi T\sum_{\omega>0}\left(F_1 - \frac{\Delta_1}{\omega}\right), \quad (32)$$

$$\Delta_0 l_2 + \Delta_1 l_1 + \Delta_2 l_0 = 2\pi T\sum_{\omega>0}\left(F_2 - \frac{\Delta_2}{\omega}\right). \quad (33)$$

Equations (22)–(33) form the basis of the following work. They enable us to derive the thermodynamic potential to third order in the quantity $(B_e - B_{c2})$.

We begin the discussion of these equations by considering, first of all, the differential equations (25), (26), and (28). These equations have to be solved with the boundary conditions (14). In this context the eigenfunctions of the operator $-\tfrac{1}{2}D\vec{\tilde{\partial}}_0^2$ [with boundary conditions (14)] are extremely important. These functions were discussed extensively by Eilenberger[10] and we also collect some useful relations in Appendix B. We denote these eigenfunctions by $\varphi_\lambda(\vec{r})$, i.e.,

$$-\tfrac{1}{2}D\vec{\tilde{\partial}}_0^2\varphi_\lambda(\vec{r}) = \epsilon_\lambda\varphi_\lambda(\vec{r}), \quad (34)$$

and normalize them according to

$$\langle\varphi_\lambda^*(\vec{r})\varphi_{\lambda'}(\vec{r})\rangle \equiv (1/\mathfrak{F})\int_{\text{cell}}dx\,dy\,\varphi_\lambda^*(\vec{r})\varphi_{\lambda'}(\vec{r}) = \delta_{\lambda\lambda'}. \quad (35)$$

The eigenvalues ϵ_λ are given by

$$\epsilon_\lambda = (2\lambda+1)\rho, \quad \lambda = 0, 1, 2, 3, \ldots. \quad (36)$$

There is no degeneracy of these eigenvalues because of the boundary conditions (14).

It is well known that Δ_0 in Eq. (25) is proportional to the ground state φ_0, i.e., that

$$\Delta_0(\vec{r}) = \Delta_{00}\varphi_0(\vec{r}). \quad (37)$$

Δ_{00} can be assumed to be real and positive.

From Eq. (25) it follows that

$$F_0(\vec{r},\omega) = \Delta_0(\vec{r})/(\omega+\rho). \quad (38)$$

Using the completeness of the set $\{\varphi_\lambda\}$ for functions obeying the boundary conditions (14), we rewrite Eqs. (26) and (28) as

$$F_1(\omega,\vec{r}) = \sum_{\lambda=0}^{\infty}\frac{\langle\varphi_\lambda^*R_1\rangle + \langle\varphi_\lambda^*\Delta_1\rangle}{\omega+\epsilon_\lambda}\varphi_\lambda(\vec{r}), \quad (39)$$

$$F_2(\omega,\vec{r}) = \sum_{\lambda=0}^{\infty}\frac{\langle\varphi_\lambda^*R_2\rangle + \langle\varphi_\lambda^*\Delta_2\rangle}{\omega+\epsilon_\lambda}\varphi_\lambda(\vec{r}). \quad (40)$$

We now turn our attention to the self-consistency equations (31)–(33). Equation (31) is automatically fulfilled because of the definition [Eq. (20)] of l_0. We then multiply Eq. (32) by $\Delta_0(\vec{r})$ and integrate over a unit cell. Using Eqs. (20) and (39) it is easily seen that Δ_1 drops out and we are left with

$$\langle\Delta_0^*\Delta_0\rangle l_1 = 2\pi T\sum_{\omega>0}\frac{\langle\Delta_0^*R_1\rangle}{\omega+\rho}. \quad (41)$$

From Eqs. (20), (33), and (40) it follows in a similar way that

$$\langle\Delta_0^*\Delta_0\rangle l_2 + \langle\Delta_0^*\Delta_1\rangle l_1 = 2\pi T\sum_{\omega>0}\frac{\langle\Delta_0^*R_2\rangle}{\omega+\rho}. \quad (42)$$

The right-hand side of Eq. (41) is built up with functions Δ_0 only; it is therefore an explicit equation for the determination of the amplitude of $\Delta_0(\vec{r})$. Equation (42) determines the important quantity $\langle\Delta_0^*\Delta_1\rangle$. But unfortunately this is not an explicit equation since R_2 is built up with the full F_1 and Δ_1. Consequently we have to know the quantities $\langle\varphi_\lambda^*\Delta_1\rangle$, $\lambda>0$, which follow from Eq. (32) by scalar multiplication with φ_λ^*. Using Eq. (39) we get

$$\langle\varphi_\lambda^*\Delta_1\rangle l_0 = 2\pi T\sum_{\omega>0}\left[\frac{\langle\varphi_\lambda^*R_1\rangle}{\omega+\epsilon_\lambda} + \langle\varphi_\lambda^*\Delta_1\rangle\left(\frac{1}{\omega+\epsilon_\lambda} - \frac{1}{\omega}\right)\right] \quad (43)$$

or

$$\langle\varphi_\lambda^*\Delta_1\rangle = \sum_{\omega>0}\frac{\langle\varphi_\lambda^*R_1\rangle}{\omega+\epsilon_\lambda}\left[\sum_{\omega>0}\left(\frac{1}{\omega+\rho} - \frac{1}{\omega+\epsilon_\lambda}\right)\right]^{-1}, \quad \lambda>0. \quad (44)$$

The quantities of interest are $\langle\Delta_0^*\Delta_0\rangle$ and $\langle\Delta_0^*\Delta_1\rangle$. They can be deduced from Eqs. (39), (41), (42), and (44) together with Eqs. (29) and (30). We postpone this calculation to the end of Sec. IV. Higher-order terms $\langle\Delta_\nu^*\Delta_\mu\rangle$ can be deduced in a similar way. But the evaluation of $\langle\Delta_0^*\Delta_1\rangle$ is already quite complicated and we will not go beyond this order.

We conclude this section by noting that the above method of deriving solutions of Eqs. (1)–(4) is also applicable to other situations, for instance, to a superconducting film in contact with a paramagnetic layer. The only change is that we have to reinterpret the pair-breaking parameters ρ and ρ_c and the boundary condition Eq. (14) in the appropriate way.

IV. THERMODYNAMICS

The difference between the thermodynamical potentials in the superconducting and the normal state is given by[11]

$$\phi=\int d^3r\left(\frac{|\Delta(\vec{r})|^2}{g}+4iT\sum_{\omega>0}\int_\omega^\infty d\omega'\right.$$
$$\left.\times[G^s_{\omega'}(\vec{r},\vec{r})-G^N_{\omega'}(\vec{r},\vec{r})]+\frac{1}{8\pi}[\vec{B}(\vec{r})-\vec{B}_e(\vec{r})]^2\right). \tag{45}$$

$G^s_\omega(\vec{r},\vec{r})$ and $G^N_\omega(\vec{r},\vec{r})$ denote Green's functions in the superconducting and the normal state, respectively. They are related to the quantity $G_\omega(\vec{r})$ [see Eq. (2)] according to

$$G^s_\omega(\vec{r},\vec{r})\equiv\frac{\pi N(0)}{i}G_\omega(\vec{r}),\quad G^N_\omega(\vec{r},\vec{r})=\frac{\pi N(0)}{i}, \tag{46}$$

the second part of Eq. (46) being a consequence of $G_\omega(\vec{r})\equiv 1$ in the normal state. Equation (46) follows immediately from the definition of the quantity $G_\omega(\vec{r})$ given in Ref. 6. Using Eq. (46) and the BCS cutoff

$$2\pi N(0)T\sum_{\omega>0}\frac{1}{\omega}=\frac{1}{g}+N(0)\ln\left(\frac{T_c}{T}\right), \tag{47}$$

we rewrite Eq. (45) as

$$\phi=\int d^3r\left[N(0)|\Delta(\vec{r})|^2\ln\left(\frac{T}{T_c}\right)\right.$$
$$+4\pi TN(0)\sum_{\omega>0}\int_\omega^\infty d\omega'\left(G_{\omega'}(\vec{r})+\frac{|\Delta(\vec{r})|^2}{2\omega'^2}-1\right)$$
$$\left.+\frac{1}{8\pi}[(\vec{B}_e(\vec{r})-\vec{B}(\vec{r}))]^2\right]. \tag{48}$$

Equation (45), or rather Eq. (48), has the following stationarity properties:

(i) Stationarity of ϕ with respect to $\Delta(\vec{r})$ and $\vec{A}(\vec{r})$ fixed leads to Eq. (3).

(ii) Stationarity of ϕ with respect to $\vec{A}(\vec{r})$ and $\Delta(\vec{r})$ fixed leads to Eq. (4). These relations were shown by Eilenberger.[11]

We now insert Eqs. (19) and (22) into Eq. (48) and differentiate the result with respect to λ (with $\bar{B}$ and T fixed). Using the above stationarity relations we get for $\tilde{\phi}$, the thermodynamic potential per unit volume, the following relation:

$$\frac{\partial}{\partial\lambda}\tilde{\phi}(\lambda)=N(0)\lambda\,(\langle|\Delta_0|^2\rangle+2\lambda\,\mathrm{Re}\langle\Delta_0^*\Delta_1\rangle+\cdots)$$
$$\times\frac{\partial}{\partial\lambda}(l_1\lambda+l_2\lambda^2+\cdots). \tag{49}$$

Integrating this equation with respect to λ we get

$$\tilde{\phi}(\lambda)-\tilde{\phi}(\lambda=0)=\tfrac{1}{2}N(0)l_1\langle|\Delta_0|^2\rangle\lambda^2+\tfrac{1}{3}2N(0)\,(l_2\langle|\Delta_0|^2\rangle$$
$$+l_1\,\mathrm{Re}\langle\Delta_0^*\Delta_1\rangle)\lambda^3. \tag{50a}$$

We neglect all terms which are of higher order than λ^3, i.e., $[eD(B_{c2}-\bar{B})]^3$. Consequently the factors in front of λ^2 and λ^3 in Eq. (50a) also may be expanded in terms of $(\bar{B}-B_{c2})$ and we get

$$\tilde{\phi}(\bar{B})=N(0)(eD)^2[\alpha(\bar{B}-B_{c2})^2+\tfrac{2}{3}eD\beta(B_{c2}-\bar{B})^3$$
$$+(1/k)(\bar{B}-B_{c2})^2]. \tag{50b}$$

The quantities k, α, and β are given by

$$k=8\pi e^2D^2N(0), \tag{51a}$$

$$\alpha=\tfrac{1}{2}l_1\langle|\Delta_0|^2\rangle|_{\bar{B}=B_{c2}}, \tag{51b}$$

$$\beta=\left(l_2\langle|\Delta_0|^2\rangle+l_1\,\mathrm{Re}\langle\Delta_0^*\Delta_1\rangle-\frac{3}{4}\frac{\partial}{\partial\rho}(l_1\langle|\Delta_0|^2\rangle)\right)\bigg|_{\bar{B}=B_{c2}}. \tag{51c}$$

We note that the derivative in Eq. (51c) has to be performed under condition (9). In going from Eq. (50a) to Eq. (50b) we used the relation

$$\tilde{\phi}(\lambda=0)=(1/8\pi)(\bar{B}-B_e)^2, \tag{52}$$

which follows immediately from Eq. (48) by using the expansion

$$\vec{B}(\vec{r})=\bar{B}\hat{z}+\lambda\,\mathrm{curl}\,\vec{a}_1+\cdots. \tag{53}$$

The minimum of $\tilde{\phi}(\bar{B})$ with respect to $\bar{B}$ under the condition that the shape of the unit cell is fixed and that Eq. (9) holds true is obtained from Eq. (50b). Note, however, that although Eq. (50b) has two extremal points in general, only the solution which leads to $\bar{B}=B_{c2}$ if B_e approaches B_{c2} is relevant. For this $\bar{B}$ we get

$$\bar{B}-B_e=\frac{B_{c2}-B_e}{1+(k\alpha)^{-1}}+\frac{eDk\beta}{(1+k\alpha)^3}(B_{c2}-B_e)^2. \tag{54}$$

The left-hand side of Eq. (54) is equal to $4\pi M$, where M denotes the magnetization per unit volume.

Inserting Eq. (54) into Eq. (50b) we get, for the thermodynamical potential as a function of the external parameters T and B_e,

$$\tilde{\phi}(T, B_e) = \frac{(B_{c2} - B_e)^2}{8\pi[1 + (k\alpha)^{-1}]} + \frac{(B_{c2} - B_e)^3 eDk\beta}{12\pi(1 + k\alpha)^3} . \quad (55)$$

From this the thermodynamical relation

$$\frac{\partial \tilde{\phi}}{\partial B_e} = \frac{B_e - \overline{B}}{4\pi} = - M \quad (56)$$

is recovered. Equation (55) still has to be minimized by varying the shape of the unit cell of the flux-line lattice.

We conclude this section by rewriting Eq. (53) somewhat. In Appendix A some steps in the evaluation of the quantities $\langle |\Delta_0|^2 \rangle$ and $\mathrm{Re}\langle \Delta_0^* \Delta_1 \rangle$ are presented. Making use of Eq. (A5) we express the quantity $l_1 \langle |\Delta_0|^2 \rangle$ and its derivative in terms of the function l_ν defined in Eqs. (18)–(20) and we express $\mathrm{Re}\langle \Delta_0^* \Delta_1 \rangle$ by means of Eq. (A15). We arrive at the following equations:

$$-4\pi M = \frac{B_{c2}(T) - B_e}{\beta_A[2\kappa_2^2(T) - 1]} + a(T) \left(\frac{1 + \beta_A[2\kappa_2^2(T) - 1]}{\beta_A[2\kappa_2^2(T) - 1]} \right)^3 [B_{c2}(T) - B_e]^2, \quad (57)$$

$$a(T) = \frac{3eDl_2}{-l_1} \left\{ \frac{\kappa_2^2 \beta_A (l_1 l_3 / l_2^2)}{[1 + \beta_A(2\kappa_2^2 - 1)]^2} + \frac{2(2\kappa_2^2)^2}{[1 + \beta_A(2\kappa_2^2 - 1)]^3} \times \left[\frac{l_1^2}{l_2^3} \left(\frac{\rho l_5}{12} - \frac{l_4}{4} \right) \beta_B + \frac{l_1^2}{l_2^3} \gamma + \left(\frac{l_4 l_1^2}{2 l_2^3} + \frac{1}{2} - \frac{l_1 l_3}{l_2^2} \right) \right] \beta_A^2 \right\} . \quad (58)$$

The quantities β_A, β_B, and γ are defined in Eqs. (A6), (A13), and (A15b). We note that the right-hand side of Eq. (58) has to be evaluated at the critical magnetic field $B_{c2}(T)$. The parameter $\kappa_2(T)$ [cf. Eq. (A7)] was introduced by Caroli *et al.*,[8] who had already calculated the linear term in Eq. (57).

V. EVALUATION OF γ

According to Eq. (A15b), γ is given by

$$\gamma = \frac{2\pi T}{\langle |\Delta_0|^2 \rangle^3} \sum_{\omega > 0} \langle (R_{1\perp} F_{1\perp}^* + \text{c. c.} - 4e^2 D \vec{a}_1^2 |F_0|^2) \rangle . \quad (59)$$

$F_{1\perp}$ denotes the component of F_1 orthogonal to the ground state Δ_0 and fulfills the equation

$$\omega F_{1\perp} - \tfrac{1}{2} D \tilde{\vec{\partial}}_0^2 F_{1\perp} = R_{1\perp} + \Delta_{1\perp} . \quad (60)$$

The purpose of the present section is to express γ in terms of integrals over the functions φ_λ [Eq. (34)].

To begin with, we introduce the operators π_x, π_y, defined by

$$\pi_x = \frac{1}{i} \frac{\partial}{\partial x} - 2e\overline{B}y, \quad \pi_y = \frac{1}{i} \frac{\partial}{\partial y} , \quad (61)$$

as well as the quantities π_+, π_-:

$$\pi_+ = \pi_x + i\pi_y, \quad \pi_- = \pi_x - i\pi_y . \quad (62)$$

It follows that

$$[\pi_+, \pi_-] = -4e\overline{B} , \quad (63)$$

$$-\tilde{\vec{\partial}}_0^2 = \pi_+ \pi_- + 2e\overline{B} . \quad (64)$$

The vector potential $\vec{a}_1$ which is determined by Eq. (30) can be assumed to have no z component:

$$\vec{a}_1 = a_x \hat{x} + a_y \hat{y} . \quad (65)$$

We then define

$$a_\pm = a_x \pm i a_y \quad (66)$$

and get

$$i \vec{a}_1 \cdot \tilde{\partial}_0 = -\tfrac{1}{2}(a_+ \pi_- + a_- \pi_+), \quad (67)$$

$$[\pi_+, a_-] = -b, \quad (68)$$

provided that $\mathrm{div}\vec{a}_1 = 0$ is fulfilled. b denotes the magnetic field given in Eq. (A3), i.e.,

$$b = (kl_1/2eD)(|\Delta_0|^2 - \langle |\Delta_0|^2 \rangle). \quad (69)$$

We now rewrite Eq. (27) somewhat differently using the above definitions. From Eq. (27) together with Eq. (38) it follows that

$$R_1 = -\tfrac{1}{2}\omega F_0 |F_0|^2 + \tfrac{1}{4} D F_0 \vec{\partial}^2 |F_0|^2 + ieD(\tilde{\vec{\partial}}_0 \cdot \vec{a}_1 + \vec{a}_1 \cdot \tilde{\vec{\partial}}_0) F_0 . \quad (70)$$

From Eqs. (67) and (68) we get

$$R_1 = -\tfrac{1}{2}\omega F_0 |F_0|^2 + \tfrac{1}{4} D F_0 \vec{\partial}^2 |F_0|^2 - eDbF_0 - eD\pi_+ a_- F_0 . \quad (71)$$

Here we used the fact that F_0 is proportional to the ground state Δ_0, i.e., that

$$\pi_- F_0 = 0 . \quad (72)$$

The component of R_1 orthogonal to the ground state Δ_0 will be written as

$$R_{1\perp} = R_0 - eD\pi_+ a_- F_0 , \quad (73)$$

with

$$R_0 = (-\tfrac{1}{2}\omega F_0 |F_0|^2 + \tfrac{1}{4} D F_0 \vec{\partial}^2 |F_0|^2 - eDbF_0)_\perp . \quad (74)$$

Using then Eqs. (64) and (73) we rewrite Eq. (60) as

$$(\omega + \rho) F_{1\perp} + \tfrac{1}{2} D \pi_+ \pi_- F_{1\perp} = R_0 - eD\pi_+ a_- F_0 + \Delta_{1\perp} . \quad (75)$$

Now we are going to eliminate the vector potential a_- from this equation.

First of all we note that Eq. (75) has no component proportional to Δ_0, so that we can apply the operator π_- without losing any information.

We then define two new functions $\tilde{F}$ and $\tilde{\Delta}$ by means of

$$\tilde{F} = \pi_- F_{1\perp} + 2ea_- F_0 \,, \tag{76}$$

$$\tilde{\Delta} = \pi_- \Delta_{1\perp} + 2ea_- \Delta_0 \,. \tag{77}$$

Applying the operator π_- to Eq. (75) and inserting Eqs. (76) and (77) into this result we arrive at

$$(\omega+\rho)\tilde{F} + \tfrac{1}{2}D\,\pi_-\pi_+\tilde{F} = \pi_- R_0 + \tilde{\Delta} \,. \tag{78}$$

The quantity Δ_1 has to be determined self-consistently according to Eq. (32). If we apply the operator π_- to this equation and insert Eqs. (76) and (77) into this result we get

$$\tilde{\Delta} l_0 = 2\pi T \sum_{\omega>0} \left(\tilde{F} - \frac{\tilde{\Delta}}{\omega}\right) \,. \tag{79}$$

Let us express γ in terms of these new functions $\tilde{\Delta}$, $\tilde{F}$. We define a quantity $\tilde{R}_0$ by

$$\pi_+ \tilde{R}_0 = R_0 \,. \tag{80}$$

Equation (80) is solvable since R_0 is orthogonal to the ground state Δ_0. It follows from Eqs. (73) and (80) that

$$\langle F_{1\perp}^* R_{1\perp}\rangle = \langle F_{1\perp}^*(\pi_+\tilde{R}_0 - eD\pi_+ a_- F_0)\rangle$$
$$= \langle (\pi_- F_{1\perp})^* (\tilde{R}_0 - eDa_- F_0)\rangle \,. \tag{81}$$

We insert Eq. (76) into Eq. (81) and this into Eq. (59) and arrive at

$$\gamma = \frac{2\pi T}{\langle|\Delta_0|^2\rangle^3} \sum_{\omega>0} (\langle \tilde{F}^* \tilde{R}_0 + \text{c.c.}\rangle - eD\langle \tilde{F}^* a_- F_0 + \text{c.c.}\rangle$$
$$- 2e\langle \tilde{R}_0^* a_- F_0 + \text{c.c.}\rangle) \,. \tag{82}$$

The term proportional to $\vec{a}_1^2$ has canceled.

In the next step we expand Eqs. (78) and (79) in terms of the eigenfunctions φ_λ defined in Eqs. (34) and (35) using the well-known relations

$$\pi_- \varphi_\lambda = \alpha_\lambda \varphi_{\lambda-1} \,, \quad \pi_+ \varphi_{\lambda-1} = \alpha_\lambda \varphi_\lambda \,, \quad \alpha_\lambda^2 = (\epsilon_\lambda - \rho)/\tfrac{1}{2}D \,. \tag{83}$$

Let us write

$$R_0 = \sum_{\lambda=1}^{\infty} C_\lambda \varphi_\lambda \,, \quad C_\lambda = \langle \varphi_\lambda^* R_0 \rangle \,. \tag{84}$$

Solving then Eqs. (78)–(80) simultaneously we get a quantity $\tilde{R}_0$ and a self-consistent quantity $\tilde{F}$ which we insert into Eq. (82). As a result of this simple calculation we get

$$\gamma = \frac{4\pi T}{\langle|\Delta_0|^2\rangle^3} \sum_{\lambda=0}^{\infty} \left\{ \sum_{\omega>0}^{\infty} \frac{|C_{\lambda+1}|^2}{\omega+\epsilon_{\lambda+1}} + \left| \sum_{\omega>0} \frac{C_{\lambda+1}}{\omega+\epsilon_{\lambda+1}} \right|^2 \left[\sum_{\omega>0} \left(\frac{1}{\omega+\rho} - \frac{1}{\omega+\epsilon_{\lambda+1}} \right) \right]^{-1} - 2e \sum_{\omega>0} \left(\frac{C_{\lambda+1}^* \langle \varphi_\lambda^* a_- F_0 \rangle}{\alpha_{\lambda+1}} + \text{c.c.} \right) \right\} . \tag{85}$$

Now let us consider the quantity $\langle \varphi_\lambda^* a_- F_0 \rangle$ or rather $\langle \varphi_\lambda^* a_- \varphi_0 \rangle$. From Eq. (68) it follows for arbitrary λ, λ' that

$$-\langle \varphi_\lambda^* b \varphi_{\lambda'} \rangle = \langle \varphi_\lambda^* [\pi_+, a_-] \varphi_{\lambda'} \rangle$$
$$= \alpha_\lambda \langle \varphi_{\lambda-1}^* a_- \varphi_{\lambda'} \rangle - \langle \varphi_\lambda^* a_- \varphi_{\lambda'+1} \rangle \alpha_{\lambda'+1} \,. \tag{86}$$

Iterating this relation and putting $\lambda' = 0$, it is not difficult to show that the following relation must hold true:

$$\frac{\langle \varphi_\lambda^* a_- \varphi_0 \rangle}{\alpha_{\lambda+1}} = -\frac{\tfrac{1}{2}D \langle \varphi_{\lambda+1}^* b \varphi_0 \rangle}{\epsilon_\lambda + \rho} - \frac{\tfrac{1}{2}D}{\epsilon_\lambda+\rho} \sum_{\mu=1}^{\infty} \frac{\alpha_1 \cdots \alpha_\mu}{\alpha_{\lambda+2} \cdots \alpha_{\lambda+1+\mu}} \langle \varphi_{\lambda+1+\mu}^* b \varphi_\mu \rangle \,. \tag{87}$$

The series on the right-hand side of Eq. (87) is convergent for $\lambda \geq 1$. Making use of Eq. (69) we get

$$-2e \frac{\langle \varphi_\lambda^* a_- \varphi_0 \rangle}{\alpha_{\lambda+1}} = \frac{kl_1}{2} \langle |\Delta_0|^2 \rangle \times \left(\frac{\langle \varphi_{\lambda+1}^* |\varphi_0|^2 \varphi_0 \rangle}{\epsilon_{\lambda+1} - \rho} + \frac{\hat{\Sigma}_{\lambda+1}}{\epsilon_{\lambda+1} - \rho} \right) . \tag{88}$$

The quantity $\hat{\Sigma}_\lambda$ is defined by

$$\hat{\Sigma}_\lambda = \sum_{\mu=1}^{\infty} \frac{\alpha_1 \cdots \alpha_\mu}{\alpha_{\lambda+1} \cdots \alpha_{\lambda+\mu}} \langle \varphi_{\lambda+\mu}^* |\varphi_0|^2 \varphi_\mu \rangle \tag{89}$$

and depends only on the shape of the unit cell and not on the magnetic field.

Next we rewrite the quantity C_λ somewhat. Making use of Eqs. (37), (38), (69), and (74) we get

$$-\frac{2C_\lambda}{\langle|\Delta_0|^2\rangle^{3/2}} \equiv \tilde{C}_\lambda = \left(\frac{\omega}{(\omega+\rho)^3} + \frac{kl_1}{\omega+\rho} \right) m_\lambda + \frac{\tilde{m}_\lambda}{(\omega+\rho)^3} \,. \tag{90}$$

m_λ is defined by

$$m_\lambda = \langle \varphi_\lambda^* |\varphi_0|^2 \varphi_0 \rangle \,, \tag{91}$$

while $\tilde{m}_\lambda$ is given according to

$$\tilde{m}_\lambda = -\tfrac{1}{2}D \langle \varphi_\lambda^* \varphi_0 \vec{\partial}^2 |\varphi_0|^2 \rangle \,. \tag{92}$$

Inserting Eqs. (88) and (90) into Eq. (85) we get

$$\gamma = \pi T \sum_{\lambda=1}^{\infty} \left\{ \sum_{\omega>0} \frac{|\tilde{C}_\lambda(\omega)|^2}{\omega+\epsilon_\lambda} + \left| \sum_{\omega>0} \frac{\tilde{C}_\lambda(\omega)}{\omega+\epsilon_\lambda} \right|^2 \left[\sum_{\omega>0} \left(\frac{1}{\omega+\rho} - \frac{1}{\omega+\epsilon_\lambda} \right) \right]^{-1} - \sum_{\omega>0} \frac{\tilde{C}_\lambda^*(\omega) kl_1}{(\omega+\rho)(\epsilon_\lambda - \rho)} [(m_\lambda + \hat{\Sigma}_\lambda) + \text{c.c.}] \right\} . \tag{93}$$

We conclude this section with a discussion of the quantity $\tilde{m}_\lambda$ [Eq. (92)]. Performing the derivatives we get

$$\tilde{m}_\lambda = -\tfrac{1}{2} D \langle \varphi_\lambda^* \varphi_0 [\varphi_0^* \tilde{\bar{\partial}}_0^2 \varphi_0 + (\tilde{\bar{\partial}}_0^2 \varphi_0)^* \varphi_0 + 2 |\tilde{\bar{\partial}}_0 \varphi_0|^2] \rangle . \tag{94}$$

This result can be cast into the form

$$\tilde{m}_\lambda = 2\rho m_\lambda - \tfrac{1}{2} D \langle \varphi_1^* \varphi_0 | \pi_+ \varphi_0 |^2 \rangle \tag{95}$$

or with the help of Eq. (83) into

$$\tilde{m}_\lambda = 2\rho (m_\lambda - \langle \varphi_\lambda^* | \varphi_1 |^2 \varphi_0 \rangle). \tag{96}$$

The term $\langle \varphi_\lambda^* | \varphi_1 |^2 \varphi_0 \rangle$ can be evaluated with methods described in Appendix B. As a result one finds

$$\tilde{m}_\lambda = \rho (\lambda + 1) m_\lambda , \tag{97}$$

and we can derive from Eq. (90)

$$\tilde{C}_\lambda = \left(\frac{(\omega + \rho) + (\omega + \epsilon_\lambda)}{2(\omega + \rho)^3} + \frac{l_2}{2\kappa_2^2 l_1 (\omega + \rho)} \right) m_\lambda , \tag{98}$$

where we use the definition of $\kappa_2(T)$, i.e.,

$$2\kappa_2^2 = l_2 / k l_1^2 . \tag{99}$$

VI. DISCUSSION

The final result for the magnetization follows from Eqs. (57), (58), and (93). But first of all we have to insert Eq. (98) into Eq. (93). The ω sums which appear during this procedure can be expressed in terms of the functions l_ν and some new functions $L_\nu(\lambda)$ defined by

$$L_\nu(\lambda) = 2\pi T \sum_{\omega > 0} \frac{1}{(\omega + \rho)^\nu (\omega + \epsilon_\lambda)} , \quad \nu = 1, 2, 3, \ldots . \tag{100}$$

We then express k in terms of κ_2^2 [Eq. (99)] and insert γ into Eq. (58), and the result of this calculation into Eq. (57). We end up with the following result for the magnetization:

$$-4\pi M = \frac{B_{c2}(T) - B_e}{\beta_A [2\kappa_2^2(T) - 1]} + \left(\frac{S_1 [2\kappa_2^2(T) + 1] + 2S_2}{[2\kappa_2^2(T) - 1]^2} + \frac{2\kappa_2^2(T) [F_1(T) + 2\kappa_2^2(T) F_2(T)]}{[2\kappa_2^2(T) - 1]^3} \right) \frac{[B_{c2}(T) - B_e]^2}{B_{c2}(T)} . \tag{101}$$

The functions $F_1(T)$, $F_2(T)$ are given by

$$F_1(T) = \frac{2 | l_3 | \rho}{l_2} \left(S_3 + \frac{3(1 - \beta_A)}{4 \beta_A^2} \right) , \tag{102}$$

$$F_2(T) = \left(\frac{| l_1 | l_4}{4 l_2^2} + \frac{l_2}{| l_1 |} - \frac{3 | l_3 |}{2 l_2} \right) \frac{3\rho}{\beta_A} + \left(\frac{| l_1 | l_4}{4 l_2^2} - \frac{\rho l_1 l_5}{6 l_2^2} \right) \frac{3\rho\beta_B}{\beta_A^3} + \frac{\rho^2 l_1 l_5}{l_2^2} S_4 + \frac{3}{4\beta_A^3} \sum_{\lambda=1}^{\infty} | m_{2\lambda} |^2 \times \left(\frac{\rho | l_1 | L_4(2\lambda)}{l_2^2} + \frac{| l_1 | [L_2(2\lambda) + l_2]^2}{4 l_2^2 L_1(2\lambda) \lambda} - \frac{1}{\lambda} \right) , \tag{103}$$

and the quantities S_ν are defined according to

$$S_1 = \frac{3}{2\beta_A^3} \sum_{\lambda=1}^{\infty} \frac{| m_{2\lambda} |^2}{2\lambda} , \qquad S_2 = \frac{3}{2\beta_A^3} \sum_{\lambda=1}^{\infty} \frac{m_{2\lambda} \hat{\Sigma}_{2\lambda}}{2\lambda} ,$$
$$S_3 = \frac{3}{2\beta_A^3} \sum_{\lambda=1}^{\infty} (m_{2\lambda} \hat{\Sigma}_{2\lambda}) , \qquad S_4 = \frac{3}{2\beta_A^3} \sum_{\lambda=1}^{\infty} 2\lambda | m_{2\lambda} |^2 . \tag{104}$$

The two parameters β_A and β_B can be expressed in terms of $m_{2\lambda}$ as well:

$$\beta_A = m_{\lambda=0} , \quad \beta_B = \sum_{\lambda=0}^{\infty} | m_{2\lambda} |^2 . \tag{105}$$

The equation for β_B is nothing else than the completeness relation for the functions φ_λ. We note that the parameter S_4 is related to β_A and β_B according to

$$S_4 = \beta_B / 2\beta_A^3 . \tag{106}$$

The proof of this relation is similar to that for Eq. (A16). In the above equations use has been made of the fact that m_λ and $\hat{\Sigma}_\lambda$ are unequal to zero only for even λ, see Appendix B.

The parameters S_ν, as well as the quantities β_A, β_B, depend only on the shape of the unit cell. The functions F_ν depend on temperature through $\rho(T)/2\pi T$, which is a universal function of the reduced temperature $t = T/T_c$. The material parameters of the alloy enter Eq. (101) only through the well-known quantity $\kappa_2(T)$.

We have calculated the parameters S_ν and the functions $F_\nu(T)$ numerically and the results are shown in Table I and in Figs. 1 and 2, respectively. From these calculations we learn that the second-order term of the magnetization is very small, suggesting that the magnetization is quite linear for fields B_e well below B_{c2}. This general feature agrees very well with measurements of the magnetization in increasing fields.[4] The graphs in Figs. 1 and 2 show that the functions F_ν may become negative leading to a negative second-order term of the quantity $-4\pi M$ for certain values of temperature and for values of $\kappa_2(T)$ very close to $(\sqrt{2})^{-1}$. This behavior, which one would not, perhaps, expect at first sight, suggests that $-4\pi M$ decreases rapidly just above B_{c1} in such a way that if one extrapolates the slope of $-4\pi M$ at B_{c2} towards B_{c1} then $-4\pi M$ should drop below this line. We consider this sharp decrease as an indication of a very weak repulsion or perhaps even of an attraction between flux lines for these particular values

TABLE I. Parameters as explained in the text for a triangular (upper row) and a square (lower row) lattice.

β_A	β_B	$S_1 \times 10^2$	$S_2 \times 10^2$	$S_3 \times 10^2$	$S_4 \times 10$
1.160	1.423	1.251	0.847	5.133	4.563
1.180	1.497	2.133	1.005	4.971	4.551

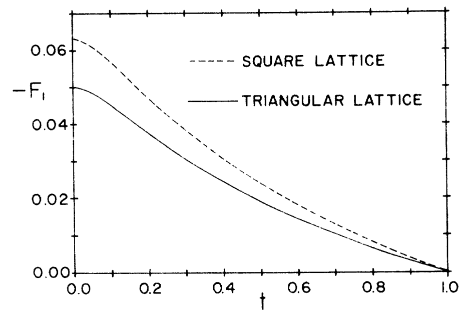

FIG. 1. $-F_1$ as a function of reduced temperature $t = T/T_c$.

of $\kappa_2(T)$.

To discuss the dependence of the magnetization on the shape of the unit cell of the flux-line lattice, we consider first the Ginzburg-Landau region. For $T \sim T_c$ we may evaluate the large parentheses in Eq. (101) at T_c, yielding

$$-4\pi M = \frac{B_{c2}(T) - B_e}{\beta_A(2\kappa^2 - 1)} + \left(\frac{S_1(2\kappa^2+1) + 2S_2}{(2\kappa^2-1)^2}\right)\frac{[B_{c2}(T) - B_e]^2}{B_{c2}(T)} , \quad (107)$$

where $\kappa \equiv \kappa_2(T_c)$. From the values in Table I it then follows that the second-order term in Eq. (107) has the tendency to reduce the difference in the magnetizations of the lattices considered. However, this does not mean that for low enough B_e the square lattice becomes the stable one. The crossover of the magnetization curves for the two lattices occurs at a field $\tilde{B}_e$ which is either smaller or just slightly bigger than the lower critical field $B_{c1}(T)$ which, in the Ginzburg-Landau region, is well known from numerical calculations.[12] Furthermore, the crossover in the thermodynamical potentials occurs at an even smaller field than $\tilde{B}_e$. Therefore, we conclude that the triangular lattice remains the stable one near T_c as far as the first- and second-order terms are concerned. For temperatures well below T_c the situation becomes more complicated. In general, the second-order term still has the tendency to decrease the difference in the magnetizations of the two lattices. For these temperatures, however, no rigorous theory for the lower critical field $B_{c1}(T)$ exists. Therefore, we are not sure, at the present time, whether the external magnetic field at which the thermodynamical potentials for the two lattices become equal lies well above $B_{c1}(T)$. However, it seems to us very unlikely that this will happen.

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APPENDIX A

In this Appendix a calculation of the quantities $\langle|\Delta_0|^2\rangle$ and $\langle \Delta_0^* \Delta_1\rangle$ is presented. We start with $\langle|\Delta_0|^2\rangle$ which is, of course, already known from the work of Caroli *et al.*[8] Combining Eqs. (27), (34), (38), and (41) we get

$$\langle|\Delta_0|^2\rangle l_1 = -\tfrac{1}{2} l_2 \langle|\Delta_0|^4\rangle - \tfrac{1}{2} l_3 \Big[\rho\langle|\Delta_0|^4\rangle + \tfrac{1}{2} D\langle|\Delta_0|^2 \vec{\partial}^2 |\Delta_0|^2\rangle - ieDl_1 \langle \vec{a}_1 \cdot (\Delta_0^* \bar{\vec{\partial}}_0 \Delta_0 - \mathrm{c.c.})\rangle\Big] . \quad (A1)$$

The vector potential $\vec{a}_1$ is determined by Eq. (29), which is rewritten as

$$\mathrm{curl\,curl}\,\vec{a}_1 = 4\pi e D N(0)(-l_1) i(\Delta_0^* \bar{\vec{\partial}}_0 \Delta_0 - \mathrm{c.c.}) . \quad (A2)$$

Making use of the well-known properties of the Abrikosov solution Δ_0, it follows that

$$\mathrm{curl}\,\vec{a}_1 \equiv \vec{b}_1 = 4\pi e D N(0) l_1 (|\Delta_0|^2 - \langle|\Delta_0|^2\rangle)\hat{z} , \quad (A3)$$

where use has been made of Eq. (13). The third term in Eq. (A1) can then be calculated easily:

$$eD(-il_1)\langle \vec{a}_1(\Delta_0^* \bar{\vec{\partial}}_0 \Delta_0 - \mathrm{c.c.})\rangle = \frac{eD}{4\pi e D N(0)} \langle \vec{a}_1 \cdot \mathrm{curl\,curl}\,\vec{a}_1\rangle . \quad (A4)$$

Making a partial integration in Eq. (A4), the surface integral of which vanishes because of Eq. (13), the third term in Eq. (A1) is expressed in terms of $\langle|\Delta_0|^4\rangle$ and $\langle|\Delta_0|^2\rangle^2$. We note that the second term in Eq. (A1) vanishes for Abrikosov solutions Δ_0. We arrive at the final answer

$$\langle|\Delta_0|^2\rangle = -\frac{2}{kl_1}[1 + \beta_A(2\kappa_2^2(T,\bar{B}) - 1)]^{-1} . \quad (A5)$$

β_A is defined by

$$\beta_A = \langle|\Delta_0|^4\rangle / (\langle|\Delta_0|^2\rangle)^2 . \quad (A6)$$

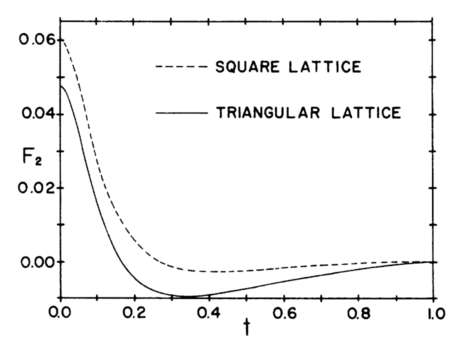

FIG. 2. F_2 as a function of reduced temperature $t = T/T_c$.

This quantity depends only on the shape of the unit cell if Eq. (9) is fulfilled. The quantity $\kappa_2(T,\bar{B})$ is defined by

$$2\kappa_2^2(T,\bar{B})=\frac{l_2(T,\rho)}{kl_1^2(T,\rho)}\,,\quad \rho=eD\bar{B}\;. \tag{A7}$$

For $\bar{B}=B_{c2}(T)$ this quantity reduces to the $\kappa_2(T)$ introduced by Caroli *et al.*[8] But we need $\kappa_2(T,\bar{B})$ also for fields $\bar{B}$ slightly smaller than $B_{c2}(T)$ in order to perform the derivative in Eq. (54). l_1 in Eq. (A5) too has to be evaluated at the field $\bar{B}$.

Next we turn our attention to the quantity $\langle\Delta_0^*\Delta_1\rangle$, or rather its real part. We first write the right-hand side of Eq. (42) using the definition of R_2 in Eq. (28):

$$2\pi T\sum_{\omega>0}\frac{\mathrm{Re}\langle\Delta_0^*R_2\rangle}{\omega+\rho}=2\pi T\sum_{\omega>0}\langle-\tfrac{1}{4}|F_0|^2(F_0^*\Delta_1+\text{c. c.})-\tfrac{1}{8}\omega|F_0|^6-\tfrac{1}{2}\omega|F_0|^2(F_0^*F_1+\text{c. c.})$$
$$+\tfrac{1}{2}D[-\tfrac{1}{4}|F_0|^2(F_0^*\tilde{\vec\partial}_0^2F_1+\text{c. c.})+\tfrac{1}{8}|F_0|^2\vec\partial^2|F_0|^4+\tfrac{3}{4}(F_0^*F_1+\text{c. c.})\vec\partial^2|F_0|^2]$$
$$+ieD\{2ie\vec{a}_1^2|F_0|^2+(\vec{a}_2-\tfrac{1}{2}|F_0|^2\vec{a}_1)(F_0^*\tilde{\vec\partial}_0F_0-\text{c. c.})+\tfrac{1}{2}\vec{a}_1[(F_0^*\tilde{\vec\partial}_0F_1+F_1^*\tilde{\vec\partial}_0F_0)-\text{c. c.}]\}\rangle\;. \tag{A8}$$

The quantities F_0 and F_1 clearly depend on ω; they are given by Eqs. (38) and (26).

We start the discussion of Eq. (A8) by noticing that the vector potential $\vec{a}_2$, which was defined in Eq. (30), enters this relation. Fortunately enough, however, we do not have to solve Eq. (30); we can eliminate $\vec{a}_2$ by means of a partial integration. From Eqs. (29) and (30) we get

$$\sum_{\omega>0}\langle\vec{a}_2(F_0^*\tilde{\vec\partial}_0F_0-\text{c. c.})\rangle=\sum_{\omega>0}\langle\vec{a}_1((F_0^*\tilde{\vec\partial}_0F_1+F_1^*\tilde{\vec\partial}_0F_0)-\text{c. c.}+4ie\vec{a}_1|F_0|^2)\rangle\;. \tag{A9}$$

Next we decompose F_1 and Δ_1 in components proportional and orthogonal to the ground state Δ_0. Combining Eq. (A8) with Eq. (42) we can then solve for $\mathrm{Re}\langle\Delta_0^*\Delta_1\rangle$.

Let us describe this procedure in some more detail. We write

$$F_1=f_1\Delta_0+F_{1\perp}\,,\quad \Delta_1=\frac{\langle\Delta_0^*\Delta_1\rangle}{\langle|\Delta_0|^2\rangle}\Delta_0+\Delta_\perp\;. \tag{A10}$$

From Eq. (39) it follows that

$$f_1=\frac{\langle F_0^*R_1\rangle}{\langle|\Delta_0|^2\rangle}+\frac{1}{\omega+\rho}\frac{\langle\Delta_0^*\Delta_1\rangle}{\langle|\Delta_0|^2\rangle}\;, \tag{A11}$$

and from Eq. (42) that

$$\mathrm{Re}\left(\frac{\langle\Delta_0^*\Delta_1\rangle}{\langle|\Delta_0|^2\rangle}\right)l_1=-l_2+\frac{2\pi T}{\langle|\Delta_0|^2\rangle}\sum_{\omega>0}\frac{\mathrm{Re}\langle\Delta_0^*R_2\rangle}{\omega+\rho}\;. \tag{A12}$$

Inserting Eqs. (A10) and (A11) into the right-hand side of Eq. (A12) [which is given by Eq. (A8)], we get first of all terms which are built up with functions Δ_0 only. These terms can be expressed by the two parameters β_A and β_B, where β_B is defined by

$$\beta_B=\langle|\Delta_0|^6\rangle/\langle|\Delta_0|^2\rangle^3\;. \tag{A13}$$

We are then left with terms containing $F_{1\perp}$, $\Delta_{1\perp}$, and $\vec{a}_1^2$. They can be simplified by using the perpendicular part of Eq. (26), i.e.,

$$\omega F_{1\perp}-\tfrac{1}{2}D\tilde{\vec\partial}_0{}^2F_{1\perp}=R_{1\perp}+\Delta_{1\perp}\,, \tag{A14}$$

to eliminate the term $\tilde{\vec\partial}_0^2F_{1\perp}$ from Eq. (A8). We get as a result of this calculation

$$\frac{-2l_1\mathrm{Re}\langle\Delta_0^*\Delta_1\rangle}{\langle|\Delta_0|^2\rangle^3}+\frac{l_2}{\langle|\Delta_0|^2\rangle^2}=\frac{3}{2}\left[\left(\frac{\rho l_5}{12}-\frac{l_4}{4}\right)\beta_B+\frac{l_4}{2}\beta_A^2-kl_1l_3\beta_A(\beta_A-1)+\frac{l_2(kl_1)^2}{2}(\beta_A-1)^2+\gamma\right]\,, \tag{A15a}$$

with

$$\gamma=\frac{2\pi T}{\langle|\Delta_0|^2\rangle^3}\sum_{\omega>0}(R_1F_{1\perp}^*+\text{c. c.}-4e^2D\vec{a}_1^2|F_0|^2)\;. \tag{A15b}$$

In deriving these equations we used the following relation, holding true for Abrikosov solutions Δ_0:

$$-\tfrac{1}{2}D\langle|\Delta_0|^2\vec\partial^2|\Delta_0|^4\rangle=\tfrac{4}{3}\rho\langle|\Delta_0|^6\rangle\;. \tag{A16}$$

To prove this relation, one first expresses the term $\vec\partial^2|\Delta_0|^4$ in terms of gauge-invariant derivations $\tilde{\vec\partial}\Delta_0$, and one can do the same for the quantity $\vec\partial^2|\Delta_0|^2$. Noticing that the left-hand side of Eq. (A16) is identical to $-\tfrac{1}{2}D\langle|\Delta_0|^4\vec\partial^2|\Delta_0|^2\rangle$ one gets two equations for this quantity from which the odd terms $|\tilde{\vec\partial}\Delta_0|^2$ can be eliminated and Eq. (A16) follows immediately.

APPENDIX B

We shall list here some important properties of the quasiperiodic eigenfunctions of the operator $\tilde{\vec\partial}_0^2$, following closely the work of Eilenberger.[10] To simplify formulas we will measure the length in units of $(2e\bar{B})^{-1/2}$. In the following the new coordinates $x/(2e\bar{B})^{1/2}$, $y/(2e\bar{B})^{1/2}$ are again written as x, y. The lattice vectors $\vec{e}_\nu$ [Eq. (11)] remain then unchanged, Eq. (9) goes over into

$$x_1 y_2 = 2\pi \ , \tag{B1}$$

and the operators π_x, π_y, $\pi_\pm$ will be replaced by

$$\pi_x = \frac{1}{i}\frac{\partial}{\partial x} - y \ , \quad \pi_y = \frac{1}{i}\frac{\partial}{\partial y} \ , \quad \pi_\pm = \pi_x \pm i\pi_y \ . \tag{B2}$$

Let us now define the function[13]

$$\varphi(\vec{r}\,|\,t) = \left(\frac{2\sqrt{\pi}}{x_1}\right)^{1/2} \times \sum_{n=-\infty}^{\infty} \exp[-\tfrac{1}{2}(y + 2t - ny_2)^2 + t^2 + iny_2(x - \tfrac{1}{2}nx_2)] \ , \tag{B3}$$

where t is a generating parameter. The following relations can be proved easily:

$$\varphi(\vec{r}\,|\,t) \text{ fulfills the boundary conditions (14),} \tag{B4a}$$

$$\pi_- \varphi(\vec{r}\,|\,0) = 0 \ , \tag{B4b}$$

$$\langle |\varphi(\vec{r}\,|0)|^2\rangle \equiv \int_{\text{cell}} |\varphi(\vec{r}_1 0)|^2 \frac{dx\,dy}{2\pi} = 1 \ , \tag{B4c}$$

$$\varphi_\lambda(\vec{r}\,|\,0) \equiv \frac{1}{(2^\lambda \lambda!)^{1/2}} (\pi_+)^\lambda \varphi(\vec{r}\,|\,0) = \frac{1}{(2^\lambda\lambda!)^{1/2}} \frac{\partial^\lambda}{\partial t^\lambda} \varphi(\vec{r}\,|\,t)\Big|_{t=0} \ , \tag{B4d}$$

$$\langle |\varphi_\lambda(\vec{r}\,|\,0)|^2\rangle \equiv 1 \ . \tag{B4e}$$

The relations (B4a)–(B4e) show that $\varphi(\vec{r}\,|\,0)$ is identical to the function $\varphi_{\lambda=0}(\vec{r})$ used in the main part of this paper. By applying the operator π_+ various times on $\varphi(\vec{r}\,|\,0)$, a set of orthogonal functions is created which fulfills the boundary conditions (14). We assume this set to be complete for functions satisfying Eq. (14). Equation (B4d) shows how this set can be derived from the generating function $\varphi(\vec{r}\,|\,t)$.

Next we introduce the function

$$\tilde{\varphi}(\vec{r}\,|\,t) = \frac{(2\pi)^{1/4}}{x_1^{1/2}} \times \sum_{n=-\infty}^{+\infty} \exp[-(y + 2t - \tfrac{1}{2}ny_2)^2 + 2t^2 + iny_2(x - \tfrac{1}{4}nx_2)] \ , \tag{B5}$$

which is closely related to $\varphi(\vec{r}\,|\,t)$. Indeed, it corresponds to a lattice with fundamental cells of smaller size but with higher magnetic field, more precisely the lattice for $\tilde{\varphi}$ is spanned by the vectors

$$\tilde{\vec{e}} = \vec{e} \ , \quad \tilde{\vec{e}}_2 = \tfrac{1}{2}\vec{e}_2 \ , \tag{B6}$$

while the relations

$$\tilde{\pi}_- \varphi(\vec{r}, 0) = 0 \ , \quad \tilde{\pi}_\pm = \frac{1}{i}\frac{\partial}{\partial x} - 2y \pm \frac{\partial}{\partial y} \tag{B7}$$

hold true. We note two other important relations:

$$\tilde{\varphi}_\lambda(\vec{r}\,|\,0) \equiv \frac{(\tilde{\pi}_+)^\lambda}{(4^\lambda\lambda!)^{1/2}} \tilde{\varphi}(\vec{r}\,|\,0) = \frac{1}{(4^\lambda\lambda!)^{1/2}} \frac{\partial^\lambda}{\partial t^\lambda} \tilde{\varphi}(\vec{r}\,|\,t)\Big|_{t=0} \tag{B8}$$

and

$$\int_{\text{cell}} |\tilde{\varphi}_\lambda(\vec{r}\,|\,0)|^2 \frac{dx\,dy}{2\pi} = 1 \ . \tag{B9}$$

We can now formulate an addition theorem,

$$\varphi(\vec{r}+\vec{r}'\,|\,0)\varphi(\vec{r}-\vec{r}'\,|\,0) = (1/\sqrt{2}\,)[\tilde{\varphi}(\vec{r}\,|\,0)\tilde{\varphi}(\vec{r}'\,|\,0) + \tilde{\varphi}(\vec{r}+\tfrac{1}{2}\vec{e}_1\,|\,0)\tilde{\varphi}(\vec{r}'+\tfrac{1}{2}\vec{e}_1\,|\,0)] \ , \tag{B10}$$

from which the following equation can be derived:

$$\varphi(\vec{r}\,|\,t_1)\varphi(\vec{r}\,|\,t_2) = \frac{1}{\sqrt{2}}\left[\tilde{\varphi}\left(\vec{r}\,\middle|\,\frac{t_1+t_2}{2}\right)\tilde{\varphi}\left(0\,\middle|\,\frac{t_1-t_2}{2}\right) + \tilde{\varphi}\left(\vec{r}+\tfrac{1}{2}\vec{e}_1\,\middle|\,\frac{t_1+t_2}{2}\right)\tilde{\varphi}\left(\tfrac{1}{2}\vec{e}_1\,\middle|\,\frac{t_1-t_2}{2}\right)\right] . \tag{B11}$$

We note another useful relation,

$$(1/F)\int_F dx\,dy\,\tilde{\varphi}^*(\vec{r}\,|\,t)\,\tilde{\varphi}(\vec{r}+\tfrac{1}{2}\vec{e}_1\,|\,t') \to 0 \ , \tag{B12}$$

which means that the left-hand side of this equation approaches 0 if F covers the entire x, y plane.

We are now able to calculate the matrix elements introduced in Sec. V. First of all it follows from Eq. (B11) together with (B12) that

$$\int_{\text{cell}} \frac{dx\,dy}{2\pi} \varphi^*(\vec{r}\,|\,t_1)\varphi^*(\vec{r}\,|\,t_2)\varphi(\vec{r}\,|\,t_3)\varphi(\vec{r}\,|\,t_4) = \frac{1}{2}\int_{\text{cell}} \frac{dx\,dy}{2\pi}\left[\tilde{\varphi}^*\left(\vec{r}\,\middle|\,\frac{t_1+t_2}{2}\right)\tilde{\varphi}\left(\vec{r}\,\middle|\,\frac{t_3+t_4}{2}\right)\tilde{\varphi}^*\left(0\,\middle|\,\frac{t_1-t_2}{2}\right)\tilde{\varphi}\left(0\,\middle|\,\frac{t_3-t_4}{2}\right) + \tilde{\varphi}^*\left(\vec{r}+\frac{\vec{e}_1}{2}\,\middle|\,\frac{t_1+t_2}{2}\right)\tilde{\varphi}\left(\vec{r}+\frac{\vec{e}_1}{2}\,\middle|\,\frac{t_3+t_4}{2}\right)\tilde{\varphi}\left(\frac{\vec{e}_1}{2}\,\middle|\,\frac{t_1-t_2}{2}\right)\tilde{\varphi}\left(\frac{\vec{e}_1}{2}\,\middle|\,\frac{t_3-t_4}{2}\right)\right] . \tag{B13}$$

The matrix elements in question can be created by differentiating Eq. (B13) according to the various generating parameters t_ν and by using the relations (B4c), (B9) and the fact that different $\tilde{\varphi}_\lambda(\vec{r}\,|\,0)$ are orthogonal to each other. Let us demonstrate this on the simple quantity m_λ. From Eqs. (91) and (B4d) it follows that

$$m_\lambda = \frac{1}{(2^\lambda\lambda!)^{1/2}} \int_{\text{cell}} \frac{dx\,dy}{2\pi} \frac{\partial^\lambda}{\partial t^\lambda}$$

$$\times \varphi^*(\vec{r}\,|\,t)\varphi^*(\vec{r}\,|\,0)\varphi(\vec{r}\,|\,0)\varphi(\vec{r}\,|\,0) \;. \tag{B14}$$

Using Eq. (B13) with $t_1 = t$ and $t_2 = t_3 = t_4 = 0$, we get

$$m_\lambda = \frac{1}{2(2^\lambda \lambda!)^{1/2}} \times \int_{\text{cell}} \frac{dx\,dy}{2\pi} \frac{\partial^\lambda}{\partial t^\lambda} \left[\tilde{\varphi}^*\left(\vec{r}\,\middle|\,\frac{t}{2}\right)\tilde{\varphi}(\vec{r}\,|\,0)\tilde{\varphi}^*\left(0\,\middle|\,\frac{t}{2}\right)\tilde{\varphi}(0\,|\,0) + \tilde{\varphi}^*\left(\vec{r}+\frac{\vec{e}_1}{2}\,\middle|\,\frac{t}{2}\right)\tilde{\varphi}\left(\vec{r}+\frac{\vec{e}_1}{2}\,\middle|\,0\right)\tilde{\varphi}^*\left(\frac{\vec{e}_1}{2}\,\middle|\,\frac{t}{2}\right)\tilde{\varphi}\left(\frac{\vec{e}_1}{2}\,\middle|\,0\right)\right]_{t=0} . \tag{B15}$$

Using the orthogonality of different function $\tilde{\varphi}_\lambda(\vec{r}\,|\,0)$ we see that only the quantities $\tilde{\varphi}^*(0\,|\,\frac{1}{2}t)$ and $\tilde{\varphi}^*(\frac{1}{2}\vec{e}_1\,|\,\frac{1}{2}t)$ have to be differentiated. With Eq. (B9) we then get the answer

$$m_\lambda = \frac{1}{2(2^\lambda \lambda!)^{1/2}} \times \frac{\partial^\lambda}{\partial t^\lambda}\left[\tilde{\varphi}^*\left(0\,\middle|\,\frac{t}{2}\right)\tilde{\varphi}(0\,|\,0) + \tilde{\varphi}^*\left(\frac{\vec{e}_1}{2}\,\middle|\,\frac{t}{2}\right)\tilde{\varphi}\left(\frac{\vec{e}_1}{2}\,\middle|\,0\right)\right]\Bigg|_{t=0} . \tag{B16}$$

Similar but slightly more complicated formulas are obtained for the quantities $\tilde{m}_\lambda$, $\hat{\Sigma}_\lambda$ introduced in Sec. V.

In the following we will consider only two types of lattices, the square lattice and the triangular lattice. We begin our discussion with the square lattice which is defined by

$$x_1 = y_2 = (2\pi)^{1/2} \equiv \xi \;, \quad x_2 = 0 \;. \tag{B17}$$

We are interested in the derivatives of the quantities $\tilde{\varphi}(0\,|\,\frac{1}{2}t)$ and $\tilde{\varphi}(\frac{1}{2}\vec{e}_1\,|\,\frac{1}{2}t)$ which can be derived easily from Eq. (B5). We get

$$A_\lambda(\xi) \equiv \frac{1}{(\lambda!)^{1/2}} \frac{\partial^\lambda}{\partial t^\lambda} \tilde{\varphi}\left(0\,\middle|\,\frac{t}{2}\right) = \sum_{n=-\infty}^{+\infty} e^{-(n\xi/2)^2} \frac{H_\lambda(n\xi)}{(\lambda!)^{1/2}} \;, \tag{B18}$$

$$\tilde{A}_\lambda(\xi) \equiv \frac{1}{(\lambda!)^{1/2}} \frac{\partial^\lambda}{\partial t^\lambda} \tilde{\varphi}\left(\frac{\vec{e}_1}{2}\,\middle|\,\frac{t}{2}\right) = \sum_{n=-\infty}^{+\infty} (-1)^n e^{-(n\xi/2)^2} \frac{H_\lambda(n\xi)}{(\lambda!)^{1/2}} \;. \tag{B19}$$

The quantities $H_\lambda(x)$ denote the Hermitian polynomials, normalized according to

$$H_{\lambda+1}(x) = xH_\lambda(x) - \lambda H_{\lambda-1}(x) \;, \quad H_0 = 1 \;, \quad H_1 = x \;. \tag{B20}$$

A triangular lattice is defined by

$$x_1 y_2 = 2\pi \;, \quad x_1/x_2 = 2 \;, \quad y_2/x_1 = \tfrac{1}{2}\sqrt{3} \;. \tag{B21}$$

With

$$\xi \equiv y_2 = (\sqrt{3}\,\pi)^{1/2} \;, \qquad \eta = 3^{1/4}/2^{1/2},$$

we obtain

$$A'_\lambda(\xi) \equiv \frac{1}{(\lambda!)^{1/2}} \frac{\partial^\lambda}{\partial t^\lambda} \tilde{\varphi}\left(0\,\middle|\,\frac{t}{2}\right) = (\sqrt{\eta}\,) \sum_{n=-\infty}^{+\infty} e^{-(n\xi/2)^2 - in^2\pi/4} \frac{H_\lambda(n\xi)}{(\lambda!)^{1/2}} \;, \tag{B22}$$

$$\tilde{A}'_\lambda(\xi) \equiv \frac{1}{(\lambda!)^{1/2}} \frac{\partial^\lambda}{\partial t^\lambda} \tilde{\varphi}\left(\frac{\vec{e}_1}{2}\,\middle|\,\frac{t}{2}\right) = (\sqrt{\eta}\,) \sum_{n=-\infty}^{+\infty} (-1)^n e^{-(n\xi/2)^2 - in^2\pi/4} \frac{H_\lambda(n\xi)}{(\lambda!)^{1/2}} \;. \tag{B23}$$

Only derivatives with an even λ are unequal to zero since the Hermitian polynomials are even or odd functions.

Finally we express the matrix elements from Sec. V in terms of the functions A_λ, $\tilde{A}_\lambda$. We get

$$m_\lambda = (2^\lambda)^{-1/2}\,\tfrac{1}{2}(A^*_\lambda A_0 + \tilde{A}^*_\lambda \tilde{A}_0), \quad \lambda = 0, 2, 4, \ldots \tag{B24}$$

$$\hat{\Sigma}_\lambda = m_\lambda + (2^\lambda)^{-1/2} \sum_{m=1}^{\infty} \left(\frac{\lambda!\,m!}{(\lambda+m)!}\right)^{1/2} (A^*_{\lambda+m}A_m + \tilde{A}^*_{\lambda+m}\tilde{A}_m) \;, \quad \lambda = 2, 4, \ldots \tag{B25}$$

$$\tilde{m}_\lambda = \rho(\lambda+1)m_\lambda \;, \qquad \lambda = 0, 2, 4, 6, \ldots \;. \tag{B26}$$

These relations hold true for both lattices if A_λ is interpreted as A'_λ for a triangular lattice. We note that the quantities m_λ, $\hat{\Sigma}_\lambda$, and $\tilde{m}_\lambda$ are real for both lattices. Equations (B24)–(B26) were used for the numerical calculation.

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