Abstract

Magnetic flux penetration in superconductors involves a rich variety of subtle phenomena, much of which is still poorly understood. Here these complexities are studied by formulating the Ginzburg-Landau equations as a lattice gauge theory. Their solutions are compared and contrasted with the (heuristic) Landau model of type I superconductivity, and the (perturbative) Abrikosov model for type II superconductors. Novelties arise as the continuum limit is approached, related to an effect discovered by Hofstadter. Various cautionary remarks pertinent to large-scale simulations are made.
1. Prolegomena.

Accurate prediction of magnetic flux penetration patterns in superconductors poses a formidable challenge. The pictures observed are the result of competition between several configurations which are degenerate in energy (or very nearly so). Intricate structures on many length scales can result. Moreover, the mechanics of multivortex systems have implications for elementary particle theory and cosmology, so the problem is of fairly general interest.

The underlying complexity of the situation mandates a nonperturbative approach. Here the Ginzburg-Landau equations are recast as a lattice gauge theory, and magnetic flux penetration patterns are determined. Comparisons are made with the classic early models of Landau (for type I superconductors) and Abrikosov (type II superconductors). Discontinuities like those in the Hofstadter “butterfly” pattern arise while approaching the continuum limit and are discussed in depth.

2. Historical background and synopsis.

Magnetic flux penetration in superconductors has been studied for over half a century. It is thus appropriate to recapitulate some of the history of the problem as its mathematical structure is set down. Most of the results relevant to this paper stem from the efforts of three authors: Landau, Abrikosov, and Hofstadter. Their contributions are sketched as the problem unfolds.

a. Landau

The geometry of the problem considered here is the same as the one used originally \([1,2]\) by Landau in 1937. A square flat plate of superconductor is situated in the \(xy\) plane, and a perpendicular field \(H\) lies in the \(\hat{z}\) direction. The magnetic field approaches a constant at large \(z\).

This early work of Landau predated the Ginzburg-Landau equations [3] by 13 years. It missed the essential difference [4] between type I and type II superconductors and ignores important effects of flux quantization. Still, it survives as a textbook [2] model of the intermediate state in type I superconductors.

Landau predicted \([1,2]\) that the magnetic field must penetrate a square plate of what is now called a “type I superconductor” in a pattern of stripes. In the above geometry, the observed pattern in the \(xy\) plane is independent of \(x\) and periodic in \(y\) (or vice-versa), requiring a complete spontaneous breakdown of the \(\text{discrete} [x \leftrightarrow y]\) symmetry. Subsequent experimental work \([5]\) revealed that the true situation in type I superconductors is far more baroque, involving patterns on many length scales. The patterns do, how-
ever, typically possess a degree of elongation, in qualitative agreement with Landau. Indeed, if the magnetic field is applied at an oblique angle, the domain patterns align [6] in a fashion resembling his model.

A better theoretical understanding of superconductors follows from the Ginzburg-Landau formalism. The major assumption of the approach [3] is that the free energy density $f(x)$ of a superconductor has an expansion

$$f(x) = f_n + \frac{1}{2} |D\psi(x)|^2 + \frac{1}{4} (|\psi(x)|^2 - 1)^2 - 1 + \frac{1}{2} \kappa^2 H^2(x)$$

(1)

where $\psi(x)$ is the order parameter (i.e., the superconductor wave function), $H(x)$ is the magnetic field, $D = \partial + iA$ is the covariant derivative and $f_n$ is the free energy of the normal state. Units are chosen so as to measure

- $x$ in units of $\xi \equiv (\Phi_0 / 2\pi B_c^2)^{1/2}$
- $A$ in units of $\xi B_c^2$
- $f(x)$ in units of $B_c^2 / 2\pi \kappa^2$
- $H(x)$ in units of $B_c^2$

(2)

where $\xi$ is the temperature-dependent coherence length and $\Phi_0 = 2\pi\hbar c/e^*$ ($e^* = 2e$) is the elementary flux quantum. Minimization of the free energy gives its Euler equations of motion:

$$D^2 \psi + \psi - |\psi|^2 \psi = 0$$

(3a)

$$+ \kappa^2 [\partial^2 A - \partial(\partial \cdot A)] = J$$

(3b)

$$J = Im[\psi^* D\psi]$$

(3c)

Note the appearance of the Abrikosov parameter $\kappa$. This Ginzburg-Landau formalism is quite general [7] and can be derived [8] from the BCS theory.

In the present work, the Landau geometry is used exclusively. The order parameter $\psi$ and vector potential $A$ depend only on $x$ and $y$ in the deep interior of a large thick superconducting plate. By use of this geometry and current conservation, the Euler equations simplify to
\[ \partial^2 r - \frac{J^2}{r^3} + r - r^3 = 0 \]  
\[ \epsilon_{ab} \partial_a (J_b / r^2) = F \]  
\[ J_b = -\kappa^2 \epsilon_{bc} \partial_c F \]

where \( \epsilon_{ab} \) is the familiar Levi-Civita antisymmetric tensor (note that \( J_a \) can be eliminated from these equations). Here,

\[ r(x, y) = |\psi(x, y)|^{\frac{1}{2}} \]  
\[ F(x, y) = \epsilon_{ab} \partial_a A_b(x, y) \]  
\[ B(x, y) = \hat{e}_z F(x, y) \]

(both are real scalars) and all indices are two-dimensional. The microscopic flux density \( B \) is in the \( \hat{z} \) direction,

b. Abrikosov

The parameter \( \kappa \) determines whether a superconductor is type I (\( \kappa^2 < \frac{1}{2} \)) or type II (\( \kappa^2 > \frac{1}{2} \)). At the boundary point (\( \kappa^2 = \frac{1}{2} \)), a partial integral of Eqs. (4) exists, sometimes called the “Sarma” [9] or “self-dual” [10] solution:

\[ -\partial^2 \ln r = 1 - r^2 = F \]

The existence of these two types of superconductor was first postulated by Abrikosov [4]. He solved the Ginzburg-Landau equations perturbatively, taking \( r \) and \( F \) to be periodic on a rectangle of size \( (\Delta x, \Delta y) \) coherence lengths. Each rectangle is penetrated by \( \nu \) units of flux

\[ \Delta x \cdot \Delta y \cdot B \cdot \xi^2 = \nu \Phi_0 \]

where \( \nu \) is an integer and \( B \) is the \( xy \) spatial average of the microscopic flux. The Abrikosov solutions are the leading terms in an expansion in \( (B_{c2} - B) \) about the linear limit, with \( B_{c2} \) the critical field above which the material goes normal (note that \( B_{c2} \equiv 1 \) here). To second order in \( (1 - B) \), the free energy eq. (1) is
\[ f(x, y) - f_n = \frac{1}{2} \kappa^2 B^2 - \frac{1}{2} \kappa^2 (1 - B)^2/[1 + (2\kappa^2 - 1)\beta] + \cdots \] (8)

where the bar denotes \( xy \) spatial average and

\[
\begin{align*}
\beta &= \overline{r^4 (r^2)^{-2}} \\
B &= \overline{F} \\
F(x, y) &= \overline{F} - \frac{1}{2} \kappa^2 [r^2(x, y) - \overline{r^2}] + \cdots
\end{align*}
\] (9)

(compare eqs. [6]).

For type II superconductors \((\kappa^2 > \frac{1}{2})\), the perturbative free energy eq. (8) is minimized when \( \beta \) is smallest,

\[ \text{Type II : } \beta = \beta_{\text{min}} \approx 1.1596 \] (10)

leading to the prediction of a triangular lattice of flux tubes \([4]\). In the type I case, \((\kappa^2 < \frac{1}{2})\), the perturbative formula eq. (8) predicts \([11-14]\) a complicated series of patterns with large \( \beta \), implying large fluctuations:

\[ \text{Type I : } \beta \approx 1/(1 - 2\kappa^2) > 1 \] (11)

Although these type I patterns are generally elongated, they differ in detail from Landau’s crude model (see 2a). The point is that the superconductor flux density \( r^2 \) behaves like a quantum “phase space” distribution \([11-12]\). The \( x \) and \( y \) coordinates of the plate are essentially Fourier conjugates, like position and momentum in quantum mechanics. The “uncertainty principle” underlying eq. (7) implies that a flux distribution which is independent of one coordinate must be sharply localized in the other, rather than the periodic function envisaged by Landau. Landau’s model of type I superconductivity is thus (oddly enough) inconsistent with the Ginzburg-Landau equations.

It is obviously imperative to go beyond the perturbative formula eq. (8). Yet a numerical simulation must confront a novel phenomenon first reported by Hofstadter \([15-17]\) and elucidated in the next section.

c. Hofstadter

The Hofstadter phenomenon becomes relevant when the Ginzburg-Landau equations are formulated on a lattice. Define complex fields \( \psi(m, n) \) and real fields \( F(m, n) \) on sites \((m, n)\) of a lattice \((x = ma, y = na; m, n = 1, \cdots, L)\)
with lattice spacing \( a \). When the partial derivatives in eqs. (3a) and (4c) are replaced by covariant differences, the resulting lattice equations are

\[
\psi(m + 1, n) + \psi(m - 1, n) + U(m, n)\psi(m, n + 1) \\
+ U^*(m, n - 1)\psi(m, n - 1) \\
= [\epsilon - a^2|\psi(m, n)|^2]\psi(m, n)
\]

(12)

\[
\kappa^2[F(m + 1, n) - F(m, n)] = J_y(m, n) \\
= Im[\psi^*(m, n)U(m, n)\psi(m, n + 1)]
\]

(13a)

\[
\kappa^2[F(m, n + 1) - F(m, n)] = -J_x(m, n) \\
= -Im[\psi^*(m, n)\psi(m + 1, n)]
\]

(13b)

\[
U(m, n) = U(m - 1, n) \times exp[ia^2F(m, n)]
\]

(13c)

where \( \epsilon \equiv 4 - a^2 \) and the gauge is chosen so that the vector potential lies in the \( y \) direction. The lattice spacing \( a \) is measured in units of the continuum coherence length. Since the desired solutions fill the \( xy \) plane, \( F \) and \( |\psi|^2 \) are taken periodic on a square of size \( L \times L \) lattice spacings. Then the periodicity of the physical currents \( J(m, n) \) implies that \( \psi \) is in general quasi-periodic rather than periodic:

\[
\psi(m, L) = \psi(m, 1) \\
\psi(L, n) = \psi(1, n) \\
\times exp[-ia^2 \sum_{m'=1}^{L} \sum_{n'=1}^{n} F(m', n')]
\]

(14)

Since \( \psi(m + L, n + L) \) is single-valued,

\[
a^2 \sum_{m=1}^{L} \sum_{n=1}^{L} F(m, n) = 2\pi p = a^2 L^2 B
\]

(15)
so \( B \) is the flux density per elementary plaquette in units of the continuum \( B_{c2} \). Here the integer \( p \) gives the number of flux quanta penetrating the \( L \times L \) large square.

Equations (12-15), though simple in appearance, imply a plethora of strange phenomena. This complexity can be illustrated by a calculation of the critical magnetic field \( B_{c2} \) on a finite lattice. When \( B \) exceeds this value, the material goes normal, and the only sensible solution to these equations is the trivial one where \( \psi(m, n) \) is vanishes. Near this limit, \( \psi(m, n) \) is small, and the nonlinear terms can be neglected. Then

\[
\begin{align*}
F_0(m, n) &= \text{constant} = B = 2\pi p/a^2 L^2 \\
U_0(m, n) &= \exp[2\pi i \frac{p}{L^2} m]
\end{align*}
\]

The equation for \( \psi(m, n) \) can be simplified by separating variables, i.e.,

\[
\psi_0(m, n) = \sum_{i=1}^{L} g_I(m) \exp[-2\pi i n L]
\]

When the nonlinear terms in eq. (12) are dropped, it becomes

\[
g_I(m + 1) + g_I(m - 1) + 2 \cos[2\pi (IL - pm)/L^2] g_I(m) = \epsilon g_I(m)
\]

which is Harper’s equation [18]. The boundary condition eq. (14) implies that

\[
g_I(m + L) = g_{I-p}(m)
\]

so that

\[
g_I(m + L^2/p) = g_I(m)
\]

(it may be necessary to define a “superlattice” [15] if \( L^2/p \) is nonintegral). Thus the natural periodicity of the \( g_I(m) \) is

\[
L^2/p \equiv 1/\alpha
\]

where \( \alpha \) is the (rational) number of flux quanta per plaquette.

The lattice bulk critical field \( B_{c2}(\alpha) \) is determined from the largest eigenvalue \( \epsilon_{\max}(\alpha) \) of eq. (18) via eq. (16):
\[ B_{c2}(\alpha) = \frac{2\pi\alpha}{[4 - \epsilon_{\text{max}}(\alpha)]} \] (21)

Note that \( B_{c2}(\alpha) \) is a function of \( \alpha \) alone.

The Hofstadter phenomenon [15] occurs when the eigenvalue spectrum of eq. (18) is calculated. The result for \( \epsilon(\alpha) \) is a very striking discontinuous “butterfly” pattern, with an intricately organized hierarchical fine structure. From eq. 15,

\[ a^2 = \left( \frac{2\pi}{B} \right) \alpha \] (22)

The continuum limit occurs when the lattice spacing approaches zero at fixed \( B \), implying that the limit of interest is \( \alpha \to 0 \). But the expected continuum limit

\[ \lim_{\alpha \to 0} B_{c2}(\alpha) = 1 \] (23)

is not obtained smoothly, instead occurring along the discontinuous upper boundary of the Hofstadter butterfly. Needless to say, this is unsettling behavior for the continuum limit of a lattice gauge theory, for presumably all thermodynamic functions (and not just \( B_{c2} \)) will display rough structure as the continuum is approached.

Two useful properties which follow from eq. (18) are

\[ \epsilon_{\text{max}}(\alpha) = \epsilon_{\text{max}}(1 - \alpha) \] (24a)

\[ \epsilon_{\text{max}}(\alpha + N) = \epsilon_{\text{max}}(\alpha) \] (24b)

where \( N \) is an arbitrary integer. Then

\[ B_{c2}(\alpha) = \frac{\alpha}{1 - \alpha} B_{c2}(1 - \alpha) \] (25)

From ref. [17] values of \( \epsilon_{\text{max}}(\alpha) \) can be extracted (see Table 1). A plot of \( B_{c2}(\alpha) \) versus \( \alpha \) is given in Fig. 1. Note that away from \( \alpha = 1/2 \).

\[ B_{c2}(\alpha) \approx 1/(1 - \alpha) \]

\[ \epsilon_{\text{max}}(\alpha) \approx 4 - 2\pi\alpha(1 - \alpha) \] (26)
(though neither is ever a continuous function) and \( B_{c2}(\alpha) \) increases without bound as \( \alpha \) approaches one. When \( \alpha = 1 \), eqs. (12) have the trivial solution

\[
\psi(m, n) = 1 \\
F(m, n) = B
\]  

(27)

[essentially equivalent to having no magnetic field, viz. eq. (24b), as \( B/B_{c2}(1) = 0 \)].

3. Numerical solution of the lattice equations.

a. Method

The lattice Ginzburg-Landau equations, eqs. (12) and (13), are readily accessible to numerical simulation [19,20], though it is well to remember the cautionary remarks of section 2c. The scheme used here is particularly simple. First, an initial choice of the \( U(m, n) \) and \( \psi(m, n) \) is made for a given average \( B \). Then eq. (12) is solved by relaxation [i.e., each of the \( \psi(m, n) \) is determined from its nearest neighbors]. One hundred sweeps through the lattice prove sufficient. Given the old \( U(m, n) \) and \( \psi(m, n) \), the new \( F(m, n) \) are determined from eq. (13) via a finite Fourier transformation in a single step with \( B \), the average of \( F(m, n) \), held fixed. The new \( U(m, n) \) are determined, and the process is repeated. Typically about 2,000 loops through the whole algorithm suffice. The usual checks using different starting conditions were made. An easy and adequate initial condition is \( F(m, n) = B \); \( \psi(m, n) = 1 \).

The limit of interest is that of small \( \alpha \), by eq. (22). Yet from eq. (20), the natural periodicity of the system is \( 1/\alpha \). Thus, \( 1/\alpha = L^2/p \geq L \). The optimal choice for \( p \) is therefore \( p = L = 1/\alpha \), and it is used here unless otherwise noted.

b. Vortex arrays in type II superconductors.

One characteristic signature of type II superconductors is the triangular lattice of flux tubes predicted by Abrikosov. The \( p \) maxima of \( F(m, n) \) per \( L \times L \) periodic square are easily seen; their patterns are displayed in fig. 2 for parameter values \( B = 0.9, \kappa^2 = 10 \) and various \( \alpha \). Since a triangular lattice involves irrational tangents, it can never fit exactly on a square lattice; yet the arrays in fig. 2 form fair approximations to a triangular lattice. In fig. 3 the squared distances \( d^2 \) between lattice points (taken in units of squared lattice spacing) are plotted versus \( 1/\alpha \) along with the Abrikosov value \( d^2 = \sqrt{4/3}/\alpha \). Reasonable agreement is obtained, though scatter is large. The
lattice spacings are equal in the $x$ and $y$ directions, so these triangular “Abrikosov” lattices are a true nonperturbative prediction (compare [20]).

For these same parameter values the $xy$ average $|\psi|^2 \equiv \rho$ is plotted versus $1/\alpha$ in fig. 4. As the $\alpha \to 0$ continuum limit is approached, the value of $\rho$ scatters discontinuously [as did $B_{c2}(\alpha)$, cf. fig. 1] but clearly approaches a limit. Comparison with continuum values thus requires fairly small $\alpha$ for respectable results. The values for $\beta(\alpha)$ [cf. eq. (10)] are much better: e.g. $\beta(1/24) = 1.1596$.

It is well to note the existence of defect structures in lattice patterns. Recall from eq. (20) that the natural periodicity of a pattern is $1/\alpha$ lattice spacings. If the system size $L$ is not an integral multiple of $1/\alpha$, defect structures due to the period mismatch can occur [fig. 5(a)]. Incomplete equilibration can also produce defects [fig. 5(b)], in this case a superimposed triangular lattice of hexagonal defects. [Other parameter values are the same as in fig. 4]. The first problem can be eliminated and the second reduced by using $p = L = 1/\alpha$.

c. $B$ versus $H$.

The difference between type I and type II superconductors can be highlighted by comparing $B$, the magnetic flux density inside the superconductor, with $H$, the applied magnetic field. Here $B$ is an input parameter given by the spatial average of $F(m,n)$, while $H$ in the present units is defined by

$$ H = \frac{1}{\kappa^2} \frac{\partial F}{\partial B} \quad (28) $$

[cf. eq. (8)] and can be calculated with an elegant virial theorem [21]. It is important to note that the assumption that $F(m,n)$ is periodic on an $L \times L$ cell implies constraints by eqs. (13),

$$ \sum_{n=1}^{L} J_y(m,n) = \sum_{n=1}^{L} J_x(m,n) = 0 \quad (29) $$

For small enough $B$, eqs. (29) are typically violated, implying that in this limit the only nontrivial solutions to the Ginzburg-Landau equations involve widely-separated magnetic vortices. Thus the plots given in fig. 6 do not continue to $B = 0$.

In fig. (6a), the type II case $\kappa^2 = 10$ is shown. Note that, as expected, $H$ is larger than $B$ and extrapolates to a finite value $H_{c1}$ as $B$ tends to zero. At the boundary point $\kappa^2 = \frac{1}{2}$ between type I and type II superconductors, [fig. (6b)]:

10
\[ H(B) = \begin{cases} B, & B > B_{c2} \\ H_{c2}, & B < B_{c2} \end{cases} \]  
while the flux patterns generated are the same as in the type II limit.

The \( B(H) \) curve for type I superconductors is more subtle. Figure (6c) displays this function for \( \kappa^2 = 0.35 \). Note that \( B(H) \) is double-valued, with turning points at \( H = H_{c2} \) and \( H = H_c > H_{c2} \). As is well-known, type I superconductors exhibit “supercooling,” leading to a hysteresis loop in the physically realized \( B(H) \). Bulk superconductors become normal at \( H = H_c \), while the normal state does not become superconducting again until \( H \) is lowered to \( H = H_{c2} < H_c \). The curve fig. 6(c) is metastable for \( B < B_{c2} \).

\[ \frac{\partial^2 f}{\partial B^2} = \kappa^2 \frac{\partial H}{\partial B} < 0 \]  
Metastability also occurs in the “effective potential” of quantum field theory and in the equation of state of thermodynamic systems (see, e.g., ref. [22]). There, as here, the proper behavior of the system can be determined by a “Landau construction,” shown as dotted lines in fig. 6(c).

The size of the metastable region is determined by the ratio \( H_c/H_{c2} \), which is \( 1/(\sqrt{2}\kappa) \) in the continuum. The metastable region thus becomes more pronounced as \( \kappa \) decreases. The Ginzburg-Landau formalism for type I superconductors [11-14] is probably only valid for \( H \) near \( H_{c2} \), and true experimental predictions for equilibrium structures are likely best obtained with “simulated annealing” methods such as that applied in [20] to type II superconductors. Flux patterns extracted from the lattice Ginzburg-Landau equations in the metastable region are generally irregular elongated nucleation lumps whose periodicity is that of the \( L \times L \) system. Thus the thickness of the superconducting plate provides an important scale [11]. Although for reasons discussed above [in sec. 2(a)] Landau’s model of flux penetration in type I superconductors is incorrect in detail, it may yet have some qualitative validity.

4. Conclusions.

As should be evident, the study of magnetic flux penetration in superconductors is a fascinating and difficult subject. Here the phenomenon was studied by formulating the Ginzburg-Landau equations as a lattice gauge theory, following a review of theoretical expectations based upon heuristic
reasoning (Landau) and perturbation theory (Abrikosov). Taking the continuum limit of the lattice gauge theory was a more subtle operation than expected, involving novelties first discussed in depth by Hofstadter.

Nevertheless, results familiar from continuum theory were readily obtained for both type I and type II superconductors. In the latter case the expected triangular “Abrikosov” lattice of flux tubes was obtained without the traditional recourse to perturbation theory.

The “intermediate state” of type I superconductors proved to be most remarkable. Here the solutions of the classical Ginzburg-Landau equations of motion were shown to predict a region of metastability, which perforce limits their domain of validity. Flux penetration in type I superconductors seems to be controlled more by the physics of metastability than by the Ginzburg-Landau paradigm, though predictions can be made [11,12]. Time-dependent theoretical [23] and experimental [24] studies should prove important here, as well as studies using “simulated annealing” methods [20].

Possible practical applications of sensitive metastable phenomena in the superconducting intermediate state include a new type of “dark matter” detector [11,12] for particle physics. It may also be useful to view intermediate state superconductors as a giant array of Josephson junctions with dynamic boundaries.

Supercomputer time provided by the Department of Energy proved useful at several stages of this work. This manuscript was typeset in LaTeX by Toni Weil.
Table 1. $\epsilon_{\text{max}}(\alpha)$ for selected $\alpha$.

| $\alpha$ | $\epsilon_{\text{max}}(\alpha)$ |
|----------|----------------------------------|
| 1/2      | $2\sqrt{2}$                      |
| 1/3      | $1 + \sqrt{3}$                   |
| 1/4      | $2\sqrt{2}$                      |
| 1/5      | 2.96645                           |
| 1/6      | $(5 + \sqrt{21})^{1/2}$           |
| 1/8      | $[6 + (12 + 8 \sqrt{2})^{1/2}]^{1/2}$ |
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Figure Captions

Figure 1
Critical field $B_{c2}(\alpha)$ versus $\alpha$ (points). The line is the function $1/(1-\alpha)$, displayed for comparison.

Figure 2
Unit cells of vortex lattices for $\kappa^2 = 10$ and $\alpha = 1/8, 1/12, 1/16, 1/20$, and $1/24$; respectively. Lines are drawn to guide the eye.

Figure 3
Squared distance (in units of $a^2$) $d^2$ between vortices plotted versus $\alpha$ for regular lattices. Dots show $d^2$ versus $1/\alpha$ (N.B. $\alpha = 10$ and 13 correspond to square lattices). Abrikosov result $\sqrt{4/3}/\alpha$ shown as straight line.

Figure 4
Average $|\psi|^2 = \rho$ versus $1/\alpha$ for $\kappa^2 = 10$ and $B = 0.90$.

Figure 5
Vortex patterns with defects (shaded).
a) $\alpha = 1/8, L = 12$  (periodicity mismatch)
b) $\alpha = 1/8, L = 16$  (insufficient equilibration).
Lines between vortices are drawn to guide the eye.

Figure 6
$B$ versus $H$ for $\alpha = 1/12$
a) $\kappa^2 = 10$
b) $\kappa^2 = 0.5$
c) $\kappa^2 = 0.35$.
Solid lines denote the calculated curve; dashed lines the “Landau construction.”