Exact solution of the Lawrence-Doniach model in parallel magnetic fields

Sergey V. Kuplevakhsy
Department of Physics, Kharkov State University, 310077 Kharkov, Ukraine

Abstract
For the first time, we obtain the complete and exact analytical solution of the Lawrence-Doniach model for layered superconductors in external parallel magnetic fields. By solving a nontrivial mathematical problem of exact minimization of the free-energy functional, we derive a closed, self-consistent system of mean-field equations involving only two variables. Exact solutions to these equations prove simultaneous penetration of Josephson vortices into all the barriers, yield a completely new expression for the lower critical field, refute the concept of a triangular Josephson vortex lattice and clarify the physics of Fraunhofer oscillations of the total critical Josephson current.

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In this paper, we obtain for the first time the complete and exact analytical solution of the popular phenomenological Lawrence-Doniach (LD) model for layered superconductors in external parallel magnetic fields.

At present, there is a universal belief that the LD model can adequately describe high-$T_c$ superconductors exhibiting the intrinsic Josephson effect. Surprisingly, despite a large number of publications on the LD model over the recent years, it has not been realized yet that in the presence of a parallel magnetic field the LD free-energy functional provides a rare example of exactly solvable models in theoretical physics. (As an exception, there is a particular exact solution of Theodorakis, valid in a restricted field range.) Moreover, even a closed, self-consistent system of mean-field equations for the LD functional has not been
obtained up until now, which in some cases leads to spurious results. Thus, calculations of
the lower critical field \[4–6\] are based on an arbitrary assumption of single Josephson vortex
penetration and a continuum approximation, incompatible with the discrete nature of the
LD model. (This treatment was criticized in Ref. 3.) The claim \[7\] that the Fraunhofer
pattern of the critical Josephson current occurs in the absence of Josephson vortices is at
odds with the well-known situation \[8\] in a single junction. Furthermore, a hypothesis \[9\] of a
triangular lattice of Josephson vortices stands in direct contradiction to the exact solution of
Ref. 3. Here we show that the origin of these inconsistencies is in an incorrect mathematical
approach to the minimization of the LD functional, neglecting principal aspects of any gauge
theory. \[10\] Based on exact variational methods, we derive a remarkably simple, closed, self-
consistent set of mean-field equations involving only two variables. As these equations
turn out to be a special limiting case of a recently developed microscopic theory, \[11\] we
concentrate here mostly on the problem of exact minimization of the LD functional and
provide a brief summary of the main new physical results at the end of the paper.

We begin by reminding basic features of the LD model. \[1,12\] In this model, the tem-
perature \(T\) is assumed to be close to the ”intrinsic” critical temperature \(T_{c0}\) of individual
layers:

\[
\tau \equiv \frac{T_{c0} - T}{T_{c0}} \ll 1. \tag{1}
\]

The superconducting (S) layers are assumed to have negligible thickness compared to the
”intrinsic” coherence length \(\zeta(T) \propto \tau^{-1/2}\); the penetration depth \(\lambda(T) \propto \tau^{-1/2}\), and the
layering period \(p\). Taking the layering axis to be \(x\), choosing the direction of the external
magnetic field \(\mathbf{H}\) to be \(z\) [\(\mathbf{H} = (0,0,H)\)] and setting \(\hbar = c = 1\), we can write the LD
free-energy functional as

\[
\Omega_{LD}\left[f_n, \phi_n, \frac{d\phi_n}{dy}, A_x, A_y; H\right] = \frac{pH^2_0(T)}{4\pi} W_z \int_{y_1}^{L_y} dy \sum_{n=-\infty}^{+\infty} \left[-f_n^2(y) + \frac{1}{2} f_n^4(y)
\right.
\]

\[
+ \zeta^2(T) \left[\frac{df_n(y)}{dy}\right]^2 + \zeta^2(T) \left[\frac{d\phi_n(y)}{dy} - 2eA_y(np, y)\right]^2 f_n^2(y)
\]

\[
+ \frac{\tau}{2} \left[f_{n-1}^2(y) + f_n^2(y) - 2f_n(y)f_{n-1}(y) \cos \Phi_{n,n-1}(y)\right]\]

\[
\int_{y_1}^{L_y} dy \sum_{n=-\infty}^{+\infty} \left[-f_n^2(y) + \frac{1}{2} f_n^4(y)
\right.
\]

\[
+ \zeta^2(T) \left[\frac{df_n(y)}{dy}\right]^2 + \zeta^2(T) \left[\frac{d\phi_n(y)}{dy} - 2eA_y(np, y)\right]^2 f_n^2(y)
\]

\[
+ \frac{\tau}{2} \left[f_{n-1}^2(y) + f_n^2(y) - 2f_n(y)f_{n-1}(y) \cos \Phi_{n,n-1}(y)\right]\]

\[
\int_{y_1}^{L_y} dy \sum_{n=-\infty}^{+\infty} \left[-f_n^2(y) + \frac{1}{2} f_n^4(y)
\right.
\]

\[
+ \zeta^2(T) \left[\frac{df_n(y)}{dy}\right]^2 + \zeta^2(T) \left[\frac{d\phi_n(y)}{dy} - 2eA_y(np, y)\right]^2 f_n^2(y)
\]

\[
+ \frac{\tau}{2} \left[f_{n-1}^2(y) + f_n^2(y) - 2f_n(y)f_{n-1}(y) \cos \Phi_{n,n-1}(y)\right]\]
\[
\frac{4e^2\zeta^2(T)\lambda^2(T)}{p} \int_{(n-1)p}^{np} dx \left[ \frac{\partial A_y(x, y)}{\partial x} - \frac{\partial A_x(x, y)}{\partial y} - H \right]^2, \tag{2}
\]

\[
\Phi_{n,n-1}(y) = \phi_n(y) - \phi_{n-1}(y) - 2e \int_{(n-1)p}^{np} dx A_x(x, y),
\]

Here \( \mathbf{A} = (A_x, A_y, 0) \) is the vector potential, continuous at the S-layers: \( \mathbf{A}(np - 0, y) = \mathbf{A}(np + 0, y) = \mathbf{A}(np, y) \); \( W_z \) is the length of the system in the \( z \) direction; \( f_n(y) \) \([0 \leq f_n(y) \leq 1]\) and \( \phi_n(y) \) are, respectively, the reduced modulus and the phase of the pair potential \( \Delta_n(y) \) in the \( n \)th superconducting layer:

\[
\Delta_n(y) = \Delta(T)f_n(y)\exp\phi_n(y), \tag{3}
\]

with \( \Delta(T) \) being the "intrinsic" gap \([\Delta(T) \propto \tau^{1/2}]\); \( H_c(T) \) is the thermodynamic critical field; \( r(T) = 2\alpha_{ph}\tau^{-1} \) is a dimensionless phenomenological parameter of the Josephson interlayer coupling \((0 < \alpha_{ph} \ll 1)\). The local magnetic field \( \mathbf{h} = (0, 0, h) \) obeys the relation

\[
h(x, y) = \frac{\partial A_y(x, y)}{\partial x} - \frac{\partial A_x(x, y)}{\partial y}. \tag{4}
\]

Our task now is to establish a closed, complete, self-consistent system of mean-field equations of the theory, which is mathematically equivalent to the minimization of (2) with respect to \( f_n, \phi_n, \) and \( \mathbf{A} \). First, we want to point out a common mistake [13] in the approach to this problem: It has not been realized in the literature that variations with respect to \( \phi_n \) and \( \mathbf{A} \) are not independent and do not yield a complete set of equations. Indeed, as the functional (4) is invariant under the gauge transformations

\[
\phi_n(y) \to \phi_n(y) + 2e\lambda(np, y), \quad A_i(x, y) \to A_i(x, y) + \partial_i\lambda(x, y), \quad i = x, y, \tag{5}
\]

where \( \lambda(x, y) \) is an arbitrary smooth function of \( x, y \) in the whole region \((-\infty < x < +\infty) \times (L_{y1} < y < L_{y2})\), variational derivatives with respect to \( \phi_n \) and \( A_x, A_y \) are related by the fundamental identities

\[
\frac{2e}{\delta\phi_n(y)} \frac{\delta\Omega_{LD}}{\delta A_y(np, y)} = \frac{\partial}{\partial y} \frac{\delta\Omega_{LD}}{\delta A_y(np, y)} + \frac{\delta\Omega_{LD}}{\delta A_y(np + 0, y)} - \frac{\delta\Omega_{LD}}{\delta A_y(np - 0, y)}. \tag{6}
\]

Being a consequence of Noether’s second theorem, such identities are typical of any gauge theory. [10] They imply that the number of independent Euler-Lagrange equations is less...
than the number of variables, and complementary relations should be imposed to eliminate irrelevant degrees of freedom and close the system mathematically. Whereas in bulk superconductors and single junctions the elimination of unphysical degrees of freedom is accomplished by fixing the gauge, in periodic weakly coupled structures this problem has additional implications. Namely, in the presence of the Josephson interlayer coupling the quantities $\Phi_{n,n-1}$ are not independent but subject to a set of constraint relations. Unfortunately, this fundamental feature was not noticed in any previous publications on the LD model.

Varying with respect to $A_x, A_y$ in the regions $(n-1)p < x < np$ under the assumption $\delta A_x(x, L_{y1}) = \delta A_x(x, L_{y2}) = 0$ yields

$$\frac{\partial h(x, y)}{\partial y} = 4\pi j_{n,n-1}(y) \equiv 4\pi j_0 f_n(y) f_{n-1}(y) \sin \Phi_{n,n-1}(y),$$

$$\frac{\partial h(x, y)}{\partial x} = 0,$$  \hspace{1cm} (7)

where $j_{n,n-1}(y)$ is the density of the Josephson current between the $(n-1)$th and the $n$th layers, $j_0 = r(T)p/16\pi \varepsilon \zeta^2(T)\lambda^2(T)$. Minimization with respect to $A_y(np, y)$ leads to boundary conditions at the S-layers:

$$h(np - 0, y) - h(np + 0, y) = \frac{pf_{n}^2(y)}{2e\lambda^2(T)} \left[ \frac{d\phi_n(y)}{dy} - 2eA_y(np, y) \right].$$

Equations (7)-(9) should be complemented by boundary conditions at the outer interfaces $y = L_{y1}, L_{y2}$. As we do not consider here externally applied currents in the $y$ direction, the first set of boundary conditions follows from the requirement $[j_{ny}]_{y=L_{y1}, L_{y2}} = 0$:

$$\left[ \frac{\partial \phi_n(x, y)}{\partial y} - 2eA_y(x, y) \right]_{y=L_{y1}, L_{y2}} = 0.$$  \hspace{1cm} (10)

Applied to Eqs. (3), these boundary conditions show that the local magnetic field at the outer interfaces is independent of the coordinate $x$: $h(x, L_{y1}) = h(L_{y1}), h(x, L_{y2}) = h(L_{y2})$. The boundary conditions imposed on $h$ should be compatible with Ampere’s law $h(L_{y2}) - h(L_{y1}) = 4\pi I$ obtained by integration of Eqs. (7) over $y$, where

$$I \equiv \int_{L_{y1}}^{L_{y2}} dy j_{n+1,n}(y) = \int_{L_{y1}}^{L_{y2}} dy j_{n,n-1}(y)$$

$$\equiv \int_{L_{y1}}^{L_{y2}} dy j_{n,n-1}(y).$$

\hspace{1cm} (11)}
is the total current in the \( x \) direction.

Differentiating (8) with respect to \( y \) and employing (7), we arrive at the current-continuity equations for the \( S \)-layers:

\[
\frac{\partial}{\partial y} \left[ f_n^2(y) \left( \frac{d\phi_n(y)}{dy} - 2eA_y(np,y) \right) \right] = \frac{r(T)}{2\zeta^2(T)} f_n(y) \left[ f_{n-1}(y) \sin \Phi_{n,n-1}(y) - f_{n+1}(y) \sin \Phi_{n+1,n}(y) \right].
\]

(12)

Adding Eqs. (12), integrating and using boundary conditions (10), we get the first integral

\[
\sum_{n=-\infty}^{+\infty} f_n^2(y) \left[ \frac{d\phi_n(y)}{dy} - 2eA_y(np,y) \right] = 0.
\]

(13)

This equation has mathematical form of a constraint relation and states that the total current in the \( y \) direction is equal to zero.

The Euler-Lagrange equations for \( \phi_n \) do not yield anything new and only reproduce Eqs. (12), as expected by virtue of Noether’s identities (8). To obtain complementary constraint relations, closing the system of the Euler-Lagrange equations and minimizing the free energy, we must modify the variational procedure.

Noting that the kinetic energy of the intralayer currents in (2) can be minimized independently of the Josephson term, we impose additional constraints

\[
\left[ \frac{\partial\phi_n(y)}{\partial y} - 2eA_y(np,y) \right] = 0,
\]

(14)

compatible with boundary conditions (14) and constraint relation (13). The requirement of compatibility with the current-conservation law (12) automatically yields another set of constraints

\[
f_{n-1}(y) \sin \Phi_{n,n-1}(y) = f_{n+1}(y) \sin \Phi_{n+1,n}(y).
\]

(15)

The physical meaning of Eqs. (14) and (15) that provide the sought necessary conditions for the true minimum of the free-energy functional (8) is obvious. Constraints (14) minimize the kinetic energy of the intralayer currents (it proves to be identically equal to zero) and assure the continuity of the local magnetic field at the \( S \)-layers: \( h(np + 0, y) = h(np - 0, y) \). [See Eq. (9)]. These constraints appear already in the case of decoupled \( S \)-layers. On the other hand, constraints (15) are uniquely imposed by the Josephson interlayer coupling.
Their function is to make the Josephson energy stationary with respect to variations of \( \phi_n \) and to assure the continuity of the Josephson current at the S-layers.

As no other conditions are imposed on the variables, we can satisfy (15) by choosing

\[
f_n(y) = f_{n-1}(y) = f(y), \quad \Phi_{n+1,n}(y) = \Phi_{n,n-1}(y) = \Phi(y).
\]  

The establishment of constraints (14)-(16), minimizing the free energy and closing the set of mean-field equations, is a key result of this paper. For example, these constraints automatically rule out any possibility of previously proposed [4] single Josephson vortex penetration and the hypothesis [9] of a triangular Josephson vortex lattice. It should be noted, however, that both the exact solution of Theodorakis [3] for the dense vortex state and early calculations [1,12,8] of the upper critical field are fully compatible with relations (14)-(16).

The remaining unphysical degree of freedom, related to the gauge invariance, is eliminated by fixing the gauge:

\[
A_x(x, y) = 0, \quad A_y(x, y) \equiv A(x, y).
\]

[Note that \( \partial A/\partial x \) and \( \partial^2 A/\partial x \partial y \) are continuous at the S-layers by virtue of (3), (14), and (3), (14).] The second set of relations (14) now yields \( \phi_n(y) = n\phi(y) + \eta(y) \), where \( \phi(y) \) is the coherent phase difference (the same at all the barriers), and \( \eta(y) \) is an arbitrary function of \( y \) that can be set equal to zero without any loss of generality.

From (8), using the continuity conditions for \( A, \partial A/\partial x \) and constraints (14), we obtain

\[
A(x, y) = \frac{1}{2e\pi} \frac{d\phi(y)}{dy} x,
\]

while the functional (2) becomes

\[
\Omega_{LD} [f, \phi; H] = \frac{H_x(T)^2}{4\pi} W_x W_z \int_{L_{y1}} f^2(y) + \frac{1}{2} f^4(y) + \zeta^2(T) \left[ \frac{df(y)}{dy} \right]^2 \]

\[
+ r(T) [1 - \cos \phi(y)] f^2(y) + 4e^2 \zeta^2(T) \lambda^2(T) \left[ \frac{1}{2e\pi} \frac{d\phi(y)}{dy} - H \right]^2,
\]

where \( W_x = L_{x2} - L_{x1} \). Minimizing (18) with respect to \( f(y) \) [with arbitrary \( \delta f(L_{y1}), \delta f(L_{y2}) \)] and \( \phi(y) \) [with \( \delta \phi(L_{y1}) = \delta \phi(L_{y2}) = 0 \)], we arrive at the desired closed, self-consistent set of mean-field equations

\[
\Delta_n(y) = \Delta f(y) \exp [in\phi(y)],
\]
that should be complemented by appropriate boundary conditions on \( h(y) \) (see above) with
\[
I \equiv \int_{L_{y1}}^{L_{y2}} dy j(y) ,
\]
where \( j(y) \) is the density of the Josephson current.

Remarkably, the coherent phase difference \( \phi \) (the same for all the barriers) obeys only one nonlinear second-order differential equation (22) with only one length scale, the Josephson penetration depth \( \lambda_J \) [Eq. (23)], as in the case of the Ferrell-Prange equation for a single junction. [14] [Mathematically, equation (22) is a solvability condition for the Maxwell equations.] Due to the factor \( f^2 \), equation (22) is coupled to nonlinear second-order differential equation (20) describing the spatial dependence of the superconducting order parameter \( f \) (the same for all the S-layers). Equations (21) constitute boundary conditions for (20). The Maxwell equations (24), (25), combined together, yield Eq. (22), as they should by virtue of self-consistency.

It is instructive to compare the above equations with those of previous publications, based on an incomplete minimization procedure. Thus, for \( \Phi_{n+1,n}(y) \) one introduces \( \Phi_{n+1,n}(y) \) an infinite non-self-consistent set of the so-called ”difference-differential” equations, containing two length scales. By virtue of the constraint relations (16), in the gauge (17) this set reduces to only one equation (22) with \( f_n(y) = 1 \), while the second length scale, \( \sqrt{2\zeta(T)/r(T)} \), related to unphysical degrees of freedom, disappears from the theory.
On the other hand, equations (19)-(25) are only a limiting case of the true microscopic equations, if one identifies \( r(T) \) with the microscopic parameter \( \alpha \zeta^2(T)/a \xi_0 \) and sets \( a/p = 0 \), where \( \xi_0 \) is the BCS coherence length, \( a \) is the S-layer thickness \( [\xi_0 \ll a \ll \zeta(T), \lambda(T)] \), and \( \alpha = \frac{3\pi^2}{\zeta(3)} \int_0^1 dtD(t) \ll 1 \) [\( D(t) \) is the tunneling probability of the barrier between two successive S-layers].

Equations (20)-(25) admit exact analytical solutions for all physical situations of interest. Aside from the region near the second-order phase transition to the normal state (because of the unphysical assumption of negligible S-layer thickness, the LD model does not adequately describe this regime [8]), these solutions stand in a one-to-one correspondence with those of the microscopic theory [11]. For this reason, we only briefly summarize the main physical results here, accentuating differences between the exact solutions and previous non-self-consistent calculations.

The local magnetic field is independent of the coordinate in the layering direction. [See Eq. (24).] The Meissner phase in semi-infinite (along the layers) samples persists up to the superheating field \( H_s = (ep\lambda J)^{-1} \). Contrary to previous suggestions, Josephson vortices penetrate all the barriers simultaneously and coherently, forming peculiar structures that we term "vortex planes". The existence of a single vortex plane in an infinite (along the layers) sample becomes energetically favorable at the lower critical field \( H_{c1\infty} = 2(\pi ep\lambda J)^{-1} \). (Previous calculations [3-4] of \( H_{c1\infty} \), based on an invalid assumption of single Josephson vortex penetration and an anisotropic continuum approximation, are incorrect.) In the fields \( H_{c1\infty} \ll H \ll [ep\zeta(T)]^{-1} \), with \( r(T) \ll 1 \), equations (20)-(25) reproduce the vortex-state solution of Theodorakis [3]. (The triangular vortex lattice [9,15] is not allowed by the exact equations.) The magnetization in the vortex state exhibits distinctive oscillatory behavior and jumps as a result of vortex-plane penetration. For a certain field range, our calculations yield a small paramagnetic effect. In contrast to previous assertions, the Fraunhofer pattern for the total critical Josephson current in layered superconductors with \( W \ll \lambda_J (W = L_y^2 - L_y) \) occurs due to successive penetration of the vortex planes and their pinning by the edges of the sample. The first zero of the Fraunhofer pattern corresponds to the lower critical field \( H_{c1W} = \pi/epW \) of a finite sample. Finally, for the upper critical field \( H_{c2\infty} \) in an infinite layered superconductor, equations (20)-(25) yield the well-known
results, as expected. We conclude by observing that the established relation to the microscopic theory casts light on the exact domain of validity of the LD model.
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