INTERLAYER VORTICES AND EDGE DISLOCATIONS IN HIGH TEMPERATURE SUPERCONDUCTORS

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Abstract

The interaction of an edge dislocation made of half the superconducting plane with a magnetic interlayer vortex is considered within the framework of the Lawrence-Doniach model with negative as well as positive Josephson interlayer coupling. In the first case the binding energy of the vortex and the dislocation has been calculated by employing a variational procedure. The current distribution around the bound vortex turns out to be asymmetric. In the second case the dislocation carries a spontaneous magnetic half-vortex, whose binding energy with the dislocation turns out to be infinite. The half-vortex energy has been calculated by the same variational procedure. Implications of the possible presence of such half-vortices for the properties of high temperature superconductors are discussed.

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1 Introduction

Many properties of high temperature superconducting (HTS) materials are well understood within the framework of Lawrence-Doniach model [1,2] assuming Josephson type coupling between the Cu-O superconducting (SC) layers. Recently in [3] it has been proven experimentally that the current-voltage and microwave characteristics of these compounds exhibit features specific to a stack of Josephson junctions (JJ), each being 10÷15 Å thick in the c-direction [3]. To date, the LD model was widely employed (see [4-7]) to describe the behavior of interlayer magnetic vortices in an ideal layered structure.

In [8] Annett has suggested that the Josephson interlayer critical current $J_c$ might be negative, if the BCS pairing mechanism is confined within each layer and does not work between the layers. In this case the ground SC state of the LD model is characterized by the phase shift $\pi$ of the order parameter in adjacent layers. To distinguish such a state from the conventional one [1,2] and following the terminology of [9], the former and the latter will be named below as $\pi$-superconducting ground state ($\pi$-SC) and 0-superconducting ground state (0-SC), respectively. It is worth noting that several mechanisms may account for the presence of $\pi$-SC (or $J_c < 0$).

As was suggested in [9], if the tunneling between two metals is controlled by spin-flip processes, the Josephson critical current between these metals should be negative. The other mechanism causing $J_c < 0$ [10], relies on the possibility that the tunneling could occur indirectly through some intermediate state where Coulomb repulsion
excludes a double occupancy of such a state. We will not further discuss here the extent to which these mechanisms are pertinent to the interlayer tunneling in HTS compounds. Instead, we will consider how the existence of $\pi$-SC, if any, may be recognized in specific features of vortex dynamics.

The 0-SC and $\pi$-SC appear to be physically indistinguishable in an ideal infinite crystal unless a screw or edge dislocation is present [11]. Then in the case of the $\pi$-SC these should carry a spontaneous half-vortex (HV) as a consequence of the phase mismatch $\pi$, while traveling around the dislocation line. Therefore an investigation of interaction between vortices and dislocations can distinguish these two SC ground states.

In what follows we will consider the interaction of the interlayer magnetic vortex (which has no normal core) with the edge linear dislocation made of half a SC plane in the two cases (0-SC and $\pi$-SC) of the LD model.

2 Model

We will employ the LD model [1,2]. As was discussed in [2,6], because of weak interlayer coupling, the constant amplitude approximation for the in-plane order parameters can be adopted in order to describe interlayer vortices. Thus, the LD free energy functional becomes dependent on the phases $\Phi_n$ and the in-layer components of the vector potential $A_n$, $n$ labels the layers. The edge dislocation can be modeled as a line $z = 0, x = 0$ so that for $x > 0$ the conducting half plane $n = 0$ is missing
To incorporate it into the LD model it is useful to separate the contribution of the \( n = 0 \) plane. Consequently, the free energy functional without the d islocation can be written as [2]

\[
F = \int d^2r \left\{ \sum_{n=1}^{+\infty} (K_n + U^+_n) + \sum_{n=-1}^{-\infty} (K_n + U^-_n) + \frac{1}{8\pi} \int dz (\text{curl} A)^2 \right. \\
\left. + \ K_0 + U_0 \right\},
\]

where the notations are introduced as follows:

\[
K_n \equiv \frac{1}{8\pi} (\varphi_0)^2 \frac{s}{\lambda_{ab}^2} (\nabla \Phi_n + \frac{2\pi}{\varphi_0} A_n)^2,
\]

\[
U^{\pm}_n \equiv \frac{\hbar}{2e} J_c [1 - \nu \cos (\Phi_n - \Phi_{n\pm 1} - \chi_{n,n\pm 1})]
\]

\[
U_0 \equiv \frac{\hbar}{2e} J_c [2 - \nu \cos (\Phi_0 - \Phi_{-1} - \chi_{0,-1}) - \nu \cos (\Phi_{1} - \Phi_0 - \chi_{1,0})]
\]

\[
\chi_{n,n+1} \equiv \frac{2\pi}{\varphi_0} \int_n^{n+1} dz A_z.
\]

Here, the superconducting layers are infinitesimally thin and separated by insulating layers of thickness \( s \); the coordinates \( r = (x, y) \) lie in the planes, and \( z \) is directed perpendicular to the layers; \( \varphi_0 \) stands for the unit flux, \( \lambda_{ab} \) is the in-plane London penetration length, \( J_c \) is the critical interlayer current; \( \nabla \equiv (\partial_x, \partial_y), A \equiv (A_x, A_y) \).

One can see that only the last two terms of (1) contain \( \Phi_0 \).

The parameter \( \nu \) is introduced here to distinguish between the two possible states of the LD model: 0-SC (\( \nu = 1 \)) [2] and \( \pi \)-SC (\( \nu = -1 \)) [8]. In the format of (1) these two states can be converted into each other by the phase shift \( \Phi_n \rightarrow \Phi_n + \pi n \).

However, the presence of a dislocation makes such a conversion impossible.

To describe a dislocation in the \( n = 0 \) layer (FIG.1) one should replace the
Josephson (potential) energy $U_0$ by the following expression:

$$U_{0d} = \frac{\hbar}{2e} J_c \begin{cases} 
2 - \nu \cos(\Phi_0 - \Phi_{-1} - \chi_{0,-1}) - \nu \cos(\Phi_1 - \Phi_0 - \chi_{1,0}), & x < 0 \\
1 - \nu \cos(\Phi_{-1} - \Phi_1 - \chi_{-1,1}), & x > 0.
\end{cases}$$

Equation (2) signifies that to the left of the dislocation line ($x < 0$), where the plane $n = 0$ exists, the interaction with the layers $n = 1$ above and $n = -1$ below is the same as given by (1). However, to the right of this line ($x > 0$) the half-plane $n = 0$ is missing and, therefore the layer $n = 1$ appears to be coupled to the $n = -1$ with the same current $J_c$. In our model we ignore any role of the dislocation core, because its size is much smaller than the London or Josephson lengths.

If a vortex resides exactly at and along the dislocation line, the lines of current should possess the symmetry with respect to the mirror reflection in the plane $z = 0$. Therefore, no current flows along the half-plane $n = 0$. It implies that the solution for such a vortex in the gauge $A_z = 0$ obeys the conditions:

$$\nabla \Phi_0 + \frac{2\pi}{\varphi_0} A_0 = 0 \quad , \quad \Phi_1 = -\Phi_{-1} \quad .$$

Making use of these conditions, one finds that the potential energy $U_0$ in (2) should be replaced by

$$U_{0d} = \frac{\hbar}{2e} J_c \begin{cases} 
2 \left(1 - \nu \cos \frac{\Phi_s}{2}\right), & x < 0 \\
1 - \nu \cos \Phi_s, & x > 0
\end{cases} ;$$

$$\Phi_s(\mathbf{r}) \equiv \Phi_1(\mathbf{r}) - \Phi_{-1}(\mathbf{r}) \quad .$$

Assuming the system is in the 0-SC state ($\nu = 1$), the lowest energy solution can be achieved for $\Phi_s = 0$. If, however, $\nu = -1$ ($\pi$-SC), the lowest energy corresponds to
the asymptotics

\[ \Phi_s(-\infty) = \pm 2\pi \quad , \quad \Phi_s(+\infty) = \pm \pi \]  

(5)

These account for a half-flux contained in the \( z = 0 \) plane. Indeed, employing the expression [12]

\[ \varphi = \frac{\varphi_0}{2\pi} (\Phi_s(+\infty) - \Phi_s(-\infty)) \]  

(6)

for the total Josephson flux \( \varphi \), one finds that \( \varphi = \mp \varphi_0/2 \). It is worth noting that imposing the condition \( \Phi_s(+\infty) = \Phi_s(-\infty) \) instead of (5) in order to remove the HV makes (4) acquire a contribution proportional to the area either of the half-plane \( n = 0 \) or the missing part of this plane. Therefore, we conclude that a single edge dislocation in \( \pi-\text{SC} \) binds the HV with an infinite energy.

To find the energy of the HV in \( \pi-\text{SC} \) as well as that of the integer vortex in 0-SC trapped at the dislocation line, we will employ the continuum limit for all the layers but the three central ones \( n = -1, 0, 1 \). It means that the potential energy (4) is retained and the summation in (1) is replaced by integration over two regions \( z > +0 \) and \( z < -0 \). We expand

\[ \cos (\Phi_n - \Phi_{n+1} - \chi_{n,n+1}) \approx 1 - s^2 \left( \frac{\partial_z \Phi}{\varphi_0} + \frac{2\pi}{\varphi_0} A_z \right)^2 \]  

(7)

for the 0-SC and the same for the \( \pi-\text{SC} \), with the replacement \( \Phi_n \to \Phi_n + \pi n \) made. The continuum approximation turns out to be valid, as discussed in [2,4], outside of the junction where the vortex resides, as long as the relation \( \lambda_{ab}/s \gg 1 \) holds. Therefore, in the following consideration the thickness of the central junction made of two infinite layers \( n = 1, n = -1 \), with the half-plane \( n = 0 \) intervening in
between, is infinitesimal. As a result, we arrive at the functional (1) written as

\[
F = \frac{1}{8\pi} \left( \frac{\varphi_0}{2\pi} \right)^2 \int_{z<0,z>0} d^2r \, dz \left[ \frac{1}{\lambda_{ab}^2} (\nabla \Phi + \frac{2\pi}{\varphi_0} A)^2 + \frac{1}{\lambda_c^2} (\partial_z \Phi + \frac{2\pi}{\varphi_0} A_z)^2 \right]
\]

\[
+ \frac{1}{8\pi} \int d^2r \, dz \left( \text{curl} A \right)^2 + \int d^2r \, U_{0d} ,
\]

(8)

where the conditions (3) and (4), which derive from (3), are taken into account.

Variation of (8) allows one to obtain the linearized bulk equations (the problem is homogeneous in the \(y\)-direction and the gauge is \(A_z = 0\)) as follows:

\[
\frac{2\pi}{\varphi_0} \partial_z^2 A_x = \frac{1}{\lambda_{ab}^2} \left( \partial_x \Phi + \frac{2\pi}{\varphi_0} A_x \right) ,
\]

(9)

and

\[
\frac{2\pi}{\varphi_0} \partial^{2}_{xx} A_x = -\frac{1}{\lambda_c^2} \partial_z \Phi .
\]

(10)

The solution for the gauge invariant phase \(\phi = \Phi + \frac{2\pi}{\varphi_0} \eta\), where the magnetic potential \(A_x = \partial_x \eta\) is introduced, can be easily found from Eqs. (9)-(10), if one Fourier transforms along the \(x\)-axis, yielding

\[
\phi_q(z) = \begin{cases} 
\phi_q(+0) e^{-Qqz}, & z > 0 \\
\phi_q(-0) e^{Qqz}, & z < 0
\end{cases} ;
\]

(11)

\[Q_q \equiv \lambda_{ab}^{-1} (1 + \lambda_c^2 q^2) \hspace{1cm} \phi_q(+0) + \phi_q(-0) = 0 .\]

Here, \(\phi_q(+0), \phi_q(-0)\) stand for the Fourier components of the gauge invariant phase at the upper and lower edges \(z = +0, z = -0\), respectively, of the central junction.

Integrating by parts with respect to \(z\) in (8) and making use of (9)-(10) one can express the free energy in terms of the surface integration only. Taking into account
that the magnetic potential $\eta$ has no jump at $z = 0$ and that the phase does have a jump, one obtains the line energy (free energy per unit length in the $y$-direction) as

$$\varepsilon = \frac{1}{4\pi} \left( \frac{\varphi_0}{2\pi} \right)^2 \left\{ \frac{1}{4\lambda_{ab}} \sum_q \frac{q^2}{\sqrt{1 + \lambda_c^2 q^2}} |\phi_{sq}|^2 \right. $$

$$ + \frac{1}{s\lambda_c^2} \left[ \int_{-\infty}^{0} dx \left( 2 \left( 1 - \nu \cos \frac{\phi_s}{2} \right) + \int_{0}^{+\infty} dx \left( 1 - \nu \cos \phi_s \right) \right) \right] \right\}, \quad (12)$$

$$\phi_{sq} \equiv \phi_q(+0) - \phi_q(-0).$$

It is worth noting that because of the limit $\lambda_{ab}/s \gg 1$, the jump of the gauge invariant phase $\phi_{sq}$ is taken to be equal to the jump $\Phi_s$ (4) of the phase $\Phi$. In the next section we will utilize (12) to calculate the energy of an integer vortex at the dislocation line (0-SC case), and show that this energy is less than that of the vortex far from the dislocation, implying a binding of the vortex to the dislocation line.

### 3 Energy of an integer vortex bound to a dislocation

If the penetration lengths $\lambda_{ab}$ were compared to $\lambda_c$, one would have converted (12) to the conventional sine-Gordon functional for the JJ [12] making the replacement $\sqrt{1 + \lambda_c^2 q^2} \approx 1$, and $\sum_q q^2 |\phi_{sq}|^2 \to \int dx (\partial_x \phi_s)^2$ in (12). Consequently, in the $\pi$-SC the HV solution would be obtained. However, the anisotropy in our case will play an essential role, implying that (12) cannot be represented in a closed form in the physical space of one coordinate $x$: an infinite number of the gradient terms should be retained. To obtain a rigorous upper bound on the vortex energy in the 0-SC we
will employ the variational trial function:

\[
\phi_s(x) = \begin{cases} 
C_e^{\alpha kx} + B e^{\frac{\pm x}{\lambda c}}, & x < 0 \\
2\pi - C_e^{-kx} - B e^{-\frac{x}{\lambda c}}, & x > 0 
\end{cases} ; \quad (13)
\]

Here, \( \alpha, k, B_\pm \) are variational parameters. It can be seen that (13) describes a function which is continuous with its first derivative. This form of the trial function corresponds to the magnetic field pointing in the \( y \)-direction, the total flux being \( \varphi_0 \) (see (6)). The term proportional to \( \exp (\pm x/\lambda_c) \) was included to account for the fact that at large distances from the vortex the solution of (9-10) decays with such exponents along the \( x \)-axis. However, it can be shown that all the terms proportional to \( B \)'s produce a contribution into the energy as small as \( s/\lambda_{ab} \ll 1 \). Thus, in what follows, we put \( B_\pm = 0 \) in (13).

Fourier transforming (13) and substituting the result into (12), we arrive at the line energy of the vortex residing at the dislocation as

\[
\varepsilon_{1d} = \left( \frac{\varphi_0}{4\pi} \right)^2 \frac{1}{\lambda_{ab}\lambda_c} \left[ \ln (k\lambda_c) + \ln 2 - \frac{\ln \alpha}{\alpha^2 - 1} + I(\alpha) \frac{\lambda_{ab}}{s} \frac{1}{k\lambda_c} + O \left( \frac{s}{\lambda_{ab}} \right) \right] \quad (14)
\]

\[
I(\alpha) \equiv \frac{2}{\pi} \left[ \int_{0}^{\frac{\alpha\pi}{2}} du \frac{\sin u^2}{u} + \frac{2}{\alpha} \int_{0}^{\frac{\alpha\pi}{2}} du \frac{\sin u^2}{u} \right] .
\]

Minimization of (14) with respect to \( k \) gives

\[
k\lambda_c = I(\alpha) \frac{\lambda_{ab}}{s} \gg 1 . \quad (15)
\]
The energy (13) then can be written as
\[ \varepsilon_{1d} = \left( \frac{\varphi_0}{4\pi} \right)^2 \frac{1}{\lambda_{ab}\lambda_c} \left[ \ln \frac{\lambda_{ab}}{s} + 1 + \ln 2 - \frac{\ln \alpha}{\alpha^2 - 1} + \ln I(\alpha) + O\left( \frac{s}{\lambda_{ab}} \right) \right] . \] (16)

This can be minimized numerically with respect to \( \alpha \), producing
\[ \varepsilon_{1d} = \left( \frac{\varphi_0}{4\pi} \right)^2 \frac{1}{\lambda_{ab}\lambda_c} \left[ \ln \frac{\lambda_{ab}}{s} + 1.05 + O\left( \frac{s}{\lambda_{ab}} \right) \right] \] (17)
at \( \alpha = 0.85 \), suggesting an asymmetric distribution of currents about the dislocation line.

To find the vortex energy far from the dislocation one can employ the same variational function (13), where the symmetric solution (\( \alpha = 1 \)) should be looked for, and the potential energy ought to be replaced by the second line of (4) in a whole space as
\[ U_0 = \frac{h}{2e} J_c (1 - \nu \cos \phi_s) , \quad -\infty < x < +\infty . \] (18)

Then, the rigorous upper bound for the integer vortex line energy far from the dislocation is
\[ \varepsilon_1 = \left( \frac{\varphi_0}{4\pi} \right)^2 \frac{1}{\lambda_{ab}\lambda_c} \left[ \ln \frac{\lambda_{ab}}{s} + 1.24 + O\left( \frac{s}{\lambda_{ab}} \right) \right] . \] (19)

A comparison of (17) and (19) shows that the latter is higher, suggesting that the vortex binds to the dislocation. It is worth noting that the exact evaluation of the line energy of an interlayer vortex in the ideal layered crystal obtained in [4] gives
\[ \varepsilon_1 = \left( \frac{\varphi_0}{4\pi} \right)^2 \frac{1}{\lambda_{ab}\lambda_c} \left[ \ln \frac{\lambda_{ab}}{s} + 1.12 + O\left( \frac{s}{\lambda_{ab}} \right) \right] , \] (20)
which appears to be higher than the energy (17) of the integer vortex bound to
the dislocation as well. Comparing (19) and (20), we can say that the vari-
tional procedure suggested above gives a correct result in the leading logarithmic
\((\ln (\lambda_{ab}/s) \gg 1)\) approximation. At the same time, the second term in brackets
(19) turns out to be overestimated by 10% in comparison with that in (20). There-
fore, as soon as the bound vortex line energy (17) contains the same \(\ln (\lambda_{ab}/c)\), we
expect that the binding energy is considerably underestimated. This, however, can
be improved by introducing additional terms into the variational ansatz (13).

## 4 The line energy of the half-vortex in the \(\pi\)-SC.

In the case \([8]\) of the \(\pi\)-SC (\(\nu = -1\)) the lowest energy solution obeys the asymptotic
behavior (5). Therefore, the trial function can be taken in the form

\[
\phi_s(x) = \begin{cases} 
2\pi - \frac{x}{1+\alpha} e^{\alpha kx}, & x < 0 \\
\pi + \frac{\alpha x}{1+\alpha} e^{-kx}, & x > 0 
\end{cases},
\]

where the tail \(\sim \exp(\pm x/\lambda_c)\) has been omitted, as discussed in Section 3. Calcula-
tions similar to those performed above for the case \(\nu = 1\) yield the solution for the
variational parameters as

\[
\lambda_c k = 1.09 \frac{\lambda_{ab}}{s}, \quad \alpha = 0.72,
\]

and the half-vortex line energy

\[
\varepsilon_{1/2} = \frac{1}{4} \left( \frac{\phi_0}{4\pi} \right)^2 \frac{1}{\lambda_{ab} \lambda_c} \left[ \ln \frac{\lambda_{ab}}{s} + 1.21 + O\left( \frac{s}{\lambda_{ab}} \right) \right].
\]
A comparison of this result with (19) shows that in the leading logarithmic approximation \( \ln(\frac{\lambda_{ab}}{s}) \gg 1 \) the line energy of the half-vortex is 1/4 that of the integer vortex, as one would expect from estimates [2,4] where the unit flux \( \varphi_0 \) is replaced by its half \( \pm \varphi_0 / 2 \).

5 Discussion.

As was emphasized above, an integer vortex turns out to be the same in the both states \( (\nu = 1, \nu = -1) \) of the LD model. It does not allow one to distinguish these states by investigating the behavior of such a vortex unless it encounters a dislocation. In the 0-SC, where the SC order parameter in the ground state has the same sign in all the layers, the edge dislocation binds the vortex with the line energy not less than

\[
\varepsilon_b = 0.07 \left( \frac{\varphi_0}{4\pi} \right)^2 \frac{1}{\lambda_{ab}\lambda_c}.
\]  

(24)

This estimate is obtained by a comparison of the exact result (20) obtained in [4] for an interlayer vortex energy in an ideal layered crystal with the variational energy (17) for the bound integer vortex.

In the \( \pi \)-SC, where the SC order parameters in the ground state have opposite signs in adjacent layers [8], the spontaneous half-vortex exists inherently at the dislocation line. Therefore, an integer vortex approaching this dislocation will either be repelled or attracted to it, depending on the mutual orientation of the two vortices. If their moments are opposite, the integer vortex will recombine with the
half-vortex. As a result of such a process, the integer vortex disappears, and the half-vortex switches orientation. It means that the energy of the former will be released in some way.

Given these two different types of interaction of free vortices with a linear edge dislocation, the two possible states of the LD model can be distinguished by investigating the dynamics of vortices in a single HTS crystal with a density of interlayer edge dislocations less than the reciprocal area \((1/\lambda_{ab}\lambda_c)\) occupied by one vortex. Under this condition the pairs of dislocations and vortices bound to them can be considered independently of each other, and our results will apply. Thus, in the case of the 0-SC these dislocations should play a role of weak pinning centers. Therefore, after imposing and then removing an external magnetic field along the layers some residual magnetisation might be observed, because of the vortices trapped by the dislocations. Effects of thermal fluctuations and weak vortex-vortex interactions will cause this magnetisation to decay slowly with the typical time determined by the line binding energy \((24)\).

As it can be shown, in the \(\pi\)-SC the ground state of an array of half-vortices attached to dislocations in a single crystal will be antiferromagnetic. Hence, no macroscopic magnetisation is expected unless an external field along the layers is imposed. Introducing external vortices, with their density being twice less than that of the dislocations, will result in them recombining with that part of the half-vortices which have the orientation opposite to the external field. As a result, a residual magnetisation of the sample will occur. This magnetisation, which was
originally due to the integer vortices, is now produced by the half-vortices ordered ferromagnetically. With the external field removed, such a configuration is not the lowest in energy, and these half-vortices should re-orient themselves to return to their former antiferromagnetic ordering. However, to do so the half-vortex should emit an integer vortex which, then, is to be expelled from the sample. The energy required for such a process is that of the integer vortex, and, as comparison of (19), (20) with (24) shows, it is bigger than the binding energy (24) in the 0-SC by the factor of \( \ln \left( \frac{\lambda_{ab}}{s} \right) \gg 1 \). Therefore, in the \( \pi \)-SC the residual magnetisation, which is controlled by the dislocation density, should decay with a typical time constant much bigger than in the 0-SC.

The other implication of the \( \pi \)-SC was discussed in [11]. If a SC grain is in the \( \pi \)-SC and contains an odd number of dislocations, it should carry a net magnetisation \( \pm \varphi_0/2 \) because of the uncompensated half-flux. An array of such grains coupled by means of the magnetic field only would exhibit paramagnetic response. In this respect the paramagnetism of the HTS granular materials [13] might be considered as an indication of the existence of the \( \pi \)-SC. The recent observation [14] of the half-flux trapped inside a HTS ring could also indicate that the grains in this ring are in the \( \pi \)-SC, and that they are joined in such a way that the Cu-O layers form a screw-like structure, while traveling around the ring. In this case such a ring characterized by the structural chirality should develop a spontaneous half-flux.

In conclusion, we employed a variational approach to show that a single interlayer edge dislocation binds an integer interlayer (coreless) vortex, within the framework
of the LD model. The current distribution around such a bound vortex turns out to be asymmetric. Regarding the suggestion [8] of the $\pi$-type interlayer Josephson coupling, we have shown that half-vortex is attached to the dislocation line, and calculated the half-vortex line energy. The physical consequences of such a ground state were discussed.

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Figure Caption

Fig.1 Schematics of the edge dislocation made of half of the conducting plane $n = 0 \ (z = 0, x < 0, -\infty < y < +\infty)$ which is inserted between the two layers $n = \pm 1$. The axis $z$ is perpendicular to the layers far from the dislocation core, which location is indicated by the vertical bar.