Exact calculation of the vortex-antivortex interaction energy in the anisotropic three-dimensional XY model

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We have developed an exact method to calculate the vortex-antivortex interaction energy in the anisotropic three-dimensional (3D) XY model. For this calculation, dual transformation, which is already known for the 2D XY model, was extended. We found an explicit form of this interaction energy as a function of the anisotropic ratio and the separation r between the vortex and antivortex located on the same layer. The form of the interaction energy is $\ln r$ at the small r limit but is proportional to r at the opposite limit. This form of interaction energy is consistent with the upper-bound calculation using the variational method by Cataudella and Minnhagen.

I. INTRODUCTION

In studying the phase fluctuation effects of high-temperature layered superconductors, several approximations[1-5] of the vortex-antivortex interaction energy have been suggested at the level of the highly anisotropic three-dimensional (3D) XY model (from now on called the layered XY model) or the Lawrence-Doniach model.[6-8] For the bare interaction energy, Cataudella and Minnhagen[1] adopted the variational method and found the upper bound of this energy. According to their calculation, this interaction energy increases linearly with the separation between the vortex and the antivortex, which is different from the logarithmically increasing energy of the 2D XY model. This is not surprising since this energy at larger separations should be dominated by the Josephson vortex lines connecting the vor-
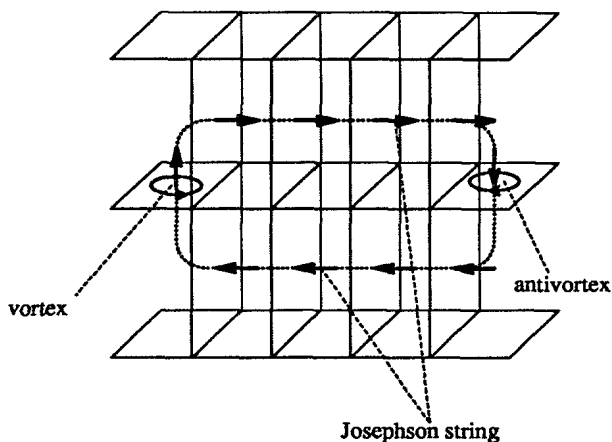

FIG. 1. Vortex-antivortex pair. In a three-dimensional lattice, a vortex line is either infinitely long or a closed loop. For a highly anisotropic three-dimensional 3D XY model, however, the above configuration is the most important. This configuration, including the Josephson string, is called a vortex-antivortex pair (Refs. 3 and 4).

tex and antivortex (see Fig. 1).

In passing, we must clarify what we mean by a vortex-antivortex pair on the same layer (Fig. 1). For the layered XY model or Lawrence-Doniach model, the vortex line cannot be disconnected, and should either be infinitely long or a closed loop. Thus a vortex and antivortex pair on a layer should be connected by Josephson vortex lines (Josephson strings) residing between the layers. Recent experimental results on high-temperature superconductors[9-15] were, however, explained through the interpretation that the phase fluctuations are associated with the layers and that major roles in phase fluctuation effects are played only by the vortex and antivortex on the layer. Hence the vortex-antivortex interaction energy is reasonably defined[3,4] as the smallest energy of the very vortex loop configuration, which corresponds to the shortest Josephson strings. The Josephson strings just modify the interaction energy of the pair at large separations. Monte Carlo simulations[3-5] performed to understand the phenomenon of vortex fluctuation at finite temperature also support this.

In the present paper we develop a dual transformation of the highly anisotropic 3D XY model and obtain an explicit form of the vortex-antivortex interaction energy as a function of the anisotropic ratio and r. The dual transformation of 2D XY model which was developed by José et al.[16] was extended for anisotropic 3D XY model. This result is compared with that of the variational calculation by Cataudella and Minnhagen.[1] We also discuss the result in connection with the high-T_c superconductors. This is under the assumption that the Lawrence-Doniach model is reduced to the layered XY model. The reduction is possible if the amplitude fluctuation is strongly suppressed and the energy associated with the induced magnetic field is neglected.[4]

II. DUAL TRANSFORMATION

We begin with the partition function

$$Z = \int_0^{2\pi} \{d\theta\} \exp\left[-\sum_{ijn} S(i|j|n)\right], \quad \{d\theta\} = \prod_{ijn} d\theta_{i,j,n},$$

$$\tag{1}$$

$$-S(i|j|n) = K_\parallel \cos\left(\theta_{i+1,j,n} - \theta_{i,j,n}\right)$$
$$+K_\parallel \cos\left(\theta_{i,j+1,n} - \theta_{i,j,n}\right)$$
$$+K_\perp \cos\left(\theta_{i,j,n+1} - \theta_{i,j,n}\right), \tag{2}$$

where $K_\parallel \equiv K$ is the intralayer coupling constant and $K_\perp \equiv \epsilon^2 K$ ($\epsilon \ll 1$) is the interlayer coupling constant. In an approximate connection to the Lawrence-Doniach model,

$$K = \frac{\hbar^2}{m}\frac{|\psi|^2}{k_B T}, \quad \epsilon^2 = \frac{m}{M}\left(\frac{\xi_\parallel}{d}\right)^2, \tag{3}$$

where ψ is the Ginzburg-Landau order parameter, and $\xi_\parallel$ is the Ginzburg-Landau in-plane coherence length. The m (M) is the effective mass parallel (perpendicular) to the plane. After expanding each exponential factor in Fourier series

$$e^{K\cos\phi} = \sum_{m=-\infty}^{\infty} I_m(K) e^{+im\phi}$$
$$\simeq I_0(K) \sum_m e^{-m^2/2K} e^{+im\phi} \quad (K \gg 1),$$

where I_m are modified Bessel functions, and after integrating out $\theta_{i,j,n}$, we can rewrite Z and S as

$$Z \propto \sum_{\{m\}}{}' \exp\left[-\sum_{ijn} S(i|j|n)\right], \tag{4}$$
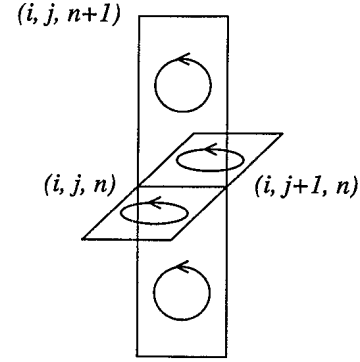

FIG. 2. Dual lattice of cubic lattice. The auxiliary field ℓ is defined at each of the face centers in the cubic lattice. The constraint of Eq. (6) to the field m is automatically satisfied for any value of the field ℓ.

$$-S(i|j|n) = -\frac{1}{2K}|m_x(i+1,i|j|n)|^2$$
$$-\frac{1}{2K}|m_y(i|j+1,j|n)|^2$$
$$-\frac{1}{2\epsilon^2 K}|m_y(i|j|n+1,n)|^2, \tag{5}$$

where the primed sum denotes the constraint

$$m_x(i+1,i|j|n) - m_x(i,i-1|j|n) + m_y(i|j+1,j|n)$$
$$-m_y(i|j,j-1|n)$$
$$+m_z(i|j|n+1,n) - m_z(i|j|n,n-1) = 0 \tag{6}$$

for all i, j, and n.

The constraint for the summation over m can be solved by moving to the dual lattice of the original cubic lattice (see Fig. 2) and by defining another integer field ℓ on the dual lattice sites

$$m_x(i,i+1|j|n) = \ell_z(i+\tfrac{1}{2}|j+\tfrac{1}{2}|n) - \ell_z(i+\tfrac{1}{2}|j-\tfrac{1}{2}|n) - \ell_y(i+\tfrac{1}{2}|j|n+\tfrac{1}{2}) + \ell_y(i+\tfrac{1}{2}|j|n-\tfrac{1}{2}),$$
$$m_y(i|j,j+1|n) = \ell_x(i|j+\tfrac{1}{2}|n+\tfrac{1}{2}) - \ell_x(i|j+\tfrac{1}{2}|n-\tfrac{1}{2}) - \ell_z(i+\tfrac{1}{2}|j+\tfrac{1}{2}|n) + \ell_z(i-\tfrac{1}{2}|j+\tfrac{1}{2}|n),$$
$$m_z(i|j|n,n+1) = \ell_y(i+\tfrac{1}{2}|j|n+\tfrac{1}{2}) - \ell_y(i-\tfrac{1}{2}|j|n+\tfrac{1}{2}) - \ell_x(i|j+\tfrac{1}{2}|n+\tfrac{1}{2}) + \ell_x(i|j-\tfrac{1}{2}|n+\tfrac{1}{2}).$$

In terms of the field on the dual lattice, Z is written in a matrix form

$$Z \propto \sum_{\{\ell\}} \exp\left[-\frac{1}{2K}\langle \ell | M | \ell \rangle\right], \tag{7}$$

where the bra and ket notation is defined below:

$$\langle \ell | M | \ell \rangle = \sum_{\mu\nu}\sum_{ii'}\sum_{jj'}\sum_{nn'} \ell_\mu(i,j,n) M_{\mu\nu}(ii'|jj'|nn')$$
$$\times \ell_\nu(i',j',n').$$

(For explicit form of M, see Appendix A.) Using the Poisson resummation rule

$$\sum_{\ell=-\infty}^{\infty} f(\ell) = \sum_{q=-\infty}^{\infty} \int_{-\infty}^{\infty} d\ell\, f(\ell) e^{2\pi i q \ell},$$

it follows that

$$Z \propto \sum_{\{Q\}} \int \{d\ell\} \exp\left[-\frac{1}{2K}\langle \ell | M | \ell \rangle + 2\pi i \langle Q(p) | \ell \rangle\right], \tag{8}$$

where the quantity Q_μ ($\mu = x, y,$ or z) is interpreted to be the vorticity in the direction of μ axes.[16]

Since the element of the matrix M depends only on the differences between the site indices, it is convenient to calculate Z in the momentum space where the matrix M is diagonal. Then we treat only the 3×3 matrix $M(p_x, p_y, p_z)$

$$Z \propto \sum_{\{Q\}} \int \{d\ell\} \exp \left[- \int (dp) S(p) \right] ,$$

$$\int (dp) = \int_0^{2\pi} \frac{d^3p}{(2\pi)^3} , \qquad (9)$$

with

$$-S(p) = -\frac{1}{2K} \langle \ell(p) \mid M(p) \mid \ell(p) \rangle + 2\pi i \langle Q(p) \mid \ell(p) \rangle . \qquad (10)$$

Now we diagonalize the matrix $M(p)$ (Appendix A) with three eigenvectors $\mid v_0 \rangle$, $\mid v_1 \rangle$, and $\mid v_2 \rangle$ and three eigenvalues $\omega_0 (= 0)$, ω_1, and ω_2. We integrate over $\langle v_0 \mid \ell \rangle$, $\langle v_1 \mid \ell \rangle$, and $\langle v_2 \mid \ell \rangle$, instead of $\mid \ell \rangle$. Then the zero eigenvalue gives a constraint to the vortex con-

figuration $\langle Q(p) \mid v_0 \rangle = 0$ or

$$Q_x(i \mid j + \tfrac{1}{2} \mid n + \tfrac{1}{2}) - Q_x(i-1 \mid j + \tfrac{1}{2} \mid n + \tfrac{1}{2}) + Q_y(i + \tfrac{1}{2} \mid j \mid n + \tfrac{1}{2})$$

$$- Q_x(i + \tfrac{1}{2} \mid j - 1 \mid n + \tfrac{1}{2})$$
$$+ Q_z(i + \tfrac{1}{2} \mid j + \tfrac{1}{2} \mid n) - Q_z(i + \tfrac{1}{2} \mid j + \tfrac{1}{2} \mid n - 1) = 0, \qquad (11)$$

i.e., the vortex line is either infinitely long or a closed loop. After Gaussian integration over $\langle v_1 \mid \ell \rangle$ and $\langle v_2 \mid \ell \rangle$, we finally obtain the partition function for vortices

$$Z \propto \sum_{\{Q\}}' \exp \left[- \int (dp) S(p) \right] \qquad (12)$$

with

$$-S(p) = -\tfrac{1}{2}(2\pi)^2 K \langle Q(p) \mid \left(\frac{1}{w_1} \mid v_1 \rangle \langle v_1 \mid + \frac{1}{w_2} \mid v_1 \rangle \langle v_2 \mid \right) \mid Q(p) \rangle , \qquad (13)$$

where the primed sum reminds us of the constraint Eq. (11).

III. RESULT

The dual transformation discussed above provides an explicit form of interaction energy of the vortex-antivortex pair on a layer (Fig. 1). Just for convenience (noting that we are interested in the large separation limit), we assume that the vortex and antivortex is placed parallel to the y axes ($Q_x = 0$). Let the separation between the vortex and the antivortex be $2r$. In this case, the configuration vector $\langle Q(p) \mid$ is given by

$$\langle Q(p) \mid = \frac{1 - e^{+i2rp_y}}{1 - e^{-ip_y}} \left(0, -[1 - e^{-ip_x}], 1 - e^{-ip_y} \right) . \qquad (14)$$

If we substitute this vector into (13), we obtain the interaction energy in units of $4\pi K$ as

$$U(2r) = \tan^{-1}(\epsilon)(2r) + \frac{2}{\pi} \int_0^{\pi/2} d\varphi \frac{\sin^2(2r\varphi)}{\sin^2 \varphi} F_\epsilon(\sin \varphi), \qquad (15)$$

where

$$F_\epsilon(\alpha) = \int_0^1 dt \left(\frac{1}{\sqrt{\epsilon^2 + 1 - t^2}} - \frac{\sqrt{1 - t^2}}{\sqrt{\alpha^2 + 1 - t^2} \sqrt{\alpha^2 + \epsilon^2 + 1 - t^2}} \right) . \qquad (16)$$

To simplify the integral form of the interaction energy of Eq. (15), we used the formula

$$\sin(2r\phi) / \sin \phi = 2 \sum_{s=1}^{r} \cos[(2s-1)\phi]. \qquad (17)$$

Note that in the case of $\epsilon = 0$, Eq. (15) is reduced into the interaction for the 2D XY model, while even a small value of ϵ induces the term linear in r.

The asymptotic expansion for $r \gg 1$ (Appendix B) gives

$$U(2r) \simeq \tan^{-1}(\epsilon)(2r) + \mu_c + \mathcal{O}(1/r) \quad (\mu_c = \text{const}). \qquad (18)$$

Cataudella and Minnhagen, in their variational calculation, took a simple approximation, where the phases on the layers next to the layer containing the vortex-antivortex pair are identically zero, and found an upper bound. Their result is expected to be larger than the values of our exact calculation. In our notations, the interaction energy of Cataudella and Minnhagen is as follows (in units of $4\pi K$):

$$U_{\text{var}}(2r) \simeq \frac{\pi}{\sqrt{2}} \epsilon (2r) + \text{const}.$$

This, compared with ours, $U(2r) \simeq [\epsilon + \mathcal{O}(\epsilon)] (2r) + \text{const}$, is larger roughly by a factor $\pi/\sqrt{2}$.

For small values of r, a simple asymptotic form is not available. But numerical evaluation shows logarithmic increase with $2r$ of the interaction energy [Fig. 3(b)]. Plots of $U(2r)$ for $2r \le 150$ and $\epsilon = 0, 0.01, 0.02, 0.03$ which include the intermediate case are shown in Fig. 3. It clearly shows crossover from logarithmic behavior for small r to linear one for large r. If the anisotropic ratio ϵ increases, the region of logarithmic dependence decreases. For the details, we draw a plot of U vs $\log_{10}(2r)$ at Fig. 3(b).

The modification of the bare vortex-antivortex interaction, in consequence, leads to the correction to the two-dimensional Berezinskii-Kosterlitz-Thouless (BKT) transition.[17-20] Hikami and Tsuneto[21] studied this effect by the renormalization group (RG) analysis. In their study, they assumed that the two-dimensional RG
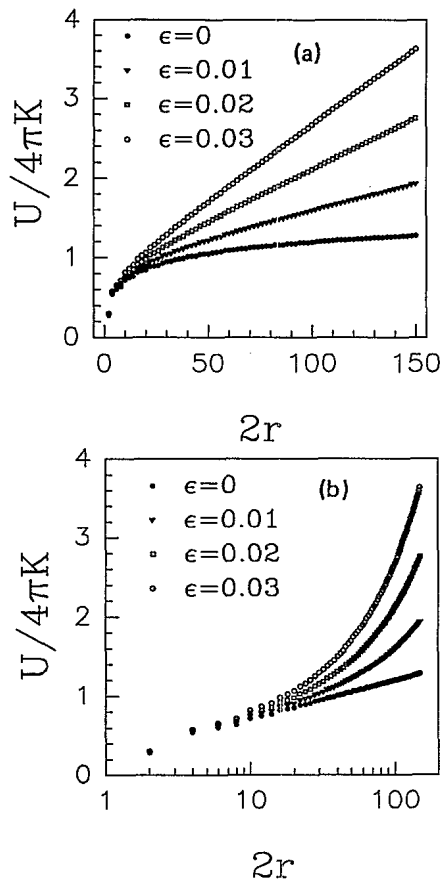
FIG. 3. Numerical evaluation of the interaction energy. Part (a) shows linear dependence on $2r$ for $r \gg 1$. At part (b), the crossover from logarithmic behavior for small r to linear behavior for large r is clear. For a comparison, the decoupled case ($\epsilon = 0$) is also plotted with filled circles.

equation[20] is valid, but subject to the cutoff $1/\epsilon$ because the vortex-antivortex interaction energy is logarithmic only at distances smaller than $1/\epsilon$ (in units of the lattice constant).[22] According to their result, for example, the true transition temperature T_c is shifted from the two-dimensional transition point T_{BKT} due to the small interlayer coupling by an amount of order $(\pi/|\ln \epsilon|)^2$. This result has also been confirmed by the Monte Carlo simulations.[3,4]

IV. CONCLUSION

We developed a dual transformation of the highly anisotropic 3D XY model to study the bare vortex-antivortex interaction. We found that this dual transformation method provides an exact form of vortex-antivortex interaction energy as a function of the anisotropic ratio and the separation between the vortex-antivortex pair. This form of this interaction is in good agreement with a zero-temperature variational calculation by Cataudella and Minnhagen. The correction to the two-dimensional BKT transition due to the small interlayer coupling was also briefly discussed.

ACKNOWLEDGMENT

APPENDIX A

In this Appendix, we summarize the information about the matrix M in Eq. (8) and Eq. (10). First we define some short-hand notations for convenience:

$$\nabla(p_\mu) = 1 - \exp(-ip_\mu),$$
$$\Delta(p_\mu) = 2(1 - \cos p_\mu), \quad \mu = x, y, \text{ or } z,$$
$$\Delta(p_x, p_y) = \Delta(p_x) + \Delta(p_y),$$
$$\Delta(p_x, p_y, p_z) = \Delta(p_x) + \Delta(p_y) + \Delta(p_z),$$
$$\Delta_\epsilon(p_x, p_y, p_z) = \Delta(p_x) + \Delta(p_y) + \epsilon^2 \Delta(p_z).$$

The Fourier transform of $M_{\mu\nu}(ii'|jj'|nn')$ is defined as

$$M_{\mu\nu}(ii'|jj'|nn') = \int (dp) \, e^{+i(i-i')p_x} e^{+i(j-j')p_y}$$
$$\times e^{+i(n-n')p_z} \, M_{\mu\nu}(p_x, p_y, p_z). \quad (A1)$$

And the momentum space 3×3 matrix $M(p_x, p_y, p_z)$ looks like

$$M = \epsilon^{-2} M_1 + M_2, \quad (A2)$$

$$M_1 = \begin{pmatrix} \Delta(p_y) & -\nabla(p_x)\nabla^*(p_y) & 0 \\ -\nabla^*(p_x)\nabla(p_y) & \Delta(p_x) & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$M_2 = \begin{pmatrix} \Delta(p_z) & 0 & -\nabla(p_x)\nabla^*(p_z) \\ 0 & 2\Delta(p_z) & -\nabla(p_y)\nabla^*(p_z) \\ -\nabla^*(p_x)\nabla(p_z) & -\nabla^*(p_y)\nabla(p_z) & \Delta(p_x, p_y) \end{pmatrix}.$$

We need eigenvalues and eigenvectors of $M(p)$. Below the eigensystem follows:

$$\omega_0 = 0, \quad \omega_1 = \Delta(p_x, p_y, p_z), \quad \omega_2 = \epsilon^{-2}\Delta_\epsilon(p_x, p_y, p_z), \quad (A3)$$

$$|\,v_0\,\rangle \propto \begin{pmatrix} \nabla(p_x) \\ \nabla(p_y) \\ \nabla(p_z) \end{pmatrix}, \quad |\,v_1\,\rangle \propto \begin{pmatrix} \nabla(p_x)\nabla^*(p_z) \\ \nabla(p_y)\nabla^*(p_z) \\ -\Delta(p_x,p_y) \end{pmatrix}, \quad |\,v_2\,\rangle \propto \begin{pmatrix} +\nabla^*(p_y) \\ -\nabla^*(p_x) \\ 0 \end{pmatrix}, \tag{A4}$$

where $|\,v_0\,\rangle$, $|\,v_1\,\rangle$, and $|\,v_2\,\rangle$ are to be normalized.

APPENDIX B

In this Appendix, we prove the asymptotic behavior in Eq. (18) of $U(2r)$ for the limit $r \gg 1$. At first, we show that the function $F_\epsilon(\alpha)$ in Eq. (16) vanishes with $\alpha \to 0$ as

$$
\begin{aligned}
F_\epsilon(\alpha) &= \alpha c \int_0^1 dt \left[\frac{\sqrt{1-t^2}}{(c^2+1-t^2)^{3/2}} + \frac{\sqrt{1-t^2}}{(c^2+\epsilon^2+1-t^2)^{3/2}} \right] \\
&\le \alpha c \int_0^1 dt \left(\frac{1}{c^2+1-t^2} + \frac{1}{c^2+\epsilon^2+1-t^2} \right) \\
&\le \alpha c \left(\frac{1}{2\sqrt{1+c^2}} \ln \frac{\sqrt{1+c^2}+1}{\sqrt{1+c^2}-1} \right) \quad (0 < c < \alpha \ll \epsilon) \\
&\le \alpha^2 \left(\frac{1}{2\sqrt{1+\alpha^2}} \ln \frac{\sqrt{1+\alpha^2}+1}{\sqrt{1+\alpha^2}-1} \right) \\
&\sim \alpha^2 |\ln \alpha|.
\end{aligned}
$$

Now we decompose $G(\alpha) \equiv F_\epsilon(\alpha)/\alpha^2$ into diverging part $G_{\text{div}}(\alpha)$ and smooth part $G_{\text{smth}}(\alpha)$. Then the above argument shows that the divergence of $G_{\text{div}}(\alpha)$ as $\alpha \to 0$ is at most logarithmic. In consequence, the integration

$$\int_0^{\pi/2} d\varphi \, \sin^2(2ry) \, |\ln \sin \varphi| = \frac{\pi}{4}\ln 2 - \frac{\pi}{8}\frac{1}{2r}$$

leads to the simple asymptotic form

$$F_\epsilon(\alpha) \le A\alpha^2 |\ln \alpha|, \quad (A > 0). \tag{B1}$$

And then, we show that for $U(2r)$, the correction to the linear behavior in r is at most $\mathcal{O}(1/r)$.

Resorting to the mean value theorem in the interval $[0,\alpha]$, there exists $0 < c < \alpha$ such that

$$F_\epsilon(\alpha) = F_\epsilon(0) + \alpha \frac{d}{dc} F_\epsilon(c).$$

Then the inequality follows:

$$\int_0^{\pi/2} d\varphi \, \sin^2(2r\varphi) G_{\text{div}}(\sin \varphi) = \text{const} + \mathcal{O}(1/r)(r \gg 1). \tag{B2}$$

Finally noting that

$$\int_0^{\pi/2} d\varphi \, \sin^2(2r\varphi) G_{\text{smth}}(\sin \varphi) = \text{const} + \mathcal{O}(1/r)(r \gg 1) \tag{B3}$$

completes the proof.

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[22] Hikami and Tsuneto assumed that $U(r) \simeq K \ln r + \epsilon^2 K r^2 + 2\mu$; quadratic instead of linear for large r. We note, however, that the cutoff factor is the same.