Vortex-phonon interaction in the Kosterlitz-Thouless theory

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The "canonical" variables of the Kosterlitz-Thouless theory—fields $\Phi_0(\mathbf{r})$ and $\varphi(\mathbf{r})$, generally believed to stand for vortices and phonons (or their *XY* equivalents, like spin waves, etc.) turn out to be neither vortices and phonons, nor, strictly speaking, *canonical* variables. The latter fact explains paradoxes of (i) absence of interaction between Φ_0 and φ, and (ii) nonphysical contribution of small vortex pairs to long-range phase correlations. We resolve the paradoxes by explicitly relating Φ_0 and φ to canonical vortex-pair and phonon variables.

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I. INTRODUCTION

Three decades ago, Kosterlitz and Thouless developed an accurate renormalization-group description of what is now called a Berezinskii-Kosterlitz-Thouless (BKT) transition[1,2]—a phase transitions in a wide class of two-dimensional systems characterized by short-range interactions and global U(1) symmetry. In accordance with the Mermin-Wagner theorem,[3,4] such systems cannot exhibit long-range order at any finite temperature. Instead, the low-temperature phase features divergent long-wave fluctuations resulting in a power-law decay of phase correlations at large distances.[1] Kosterlitz and Thouless revealed the importance of configurations with pointlike topological defects or topological charges, such as Coulomb charges in plasma, dislocations in crystals, vortices in superfluid and spin systems, etc. At low temperature, the defects exist only in the form a dilute gas of bound pairs of opposite topological charges. At higher temperature, pairs of large separation become more probable and eventual pair dissociation at critical temperature destroys the algebraic long-range order. Extensive theoretical work[1,2,5–9] provides a complete quantitative description of critical properties in such systems. The theory is corroborated by comprehensive experimental studies of ^{4}He films[10–13] and superconducting Josephson arrays.[14] Recent advances in the area of ultra-cold gases have made it possible to render BKT transition in optical lattices.[15]

The Kosterlitz-Thouless (KT) theory starts with a generic effective action[2]

$$A[\Phi] = K_0 \int |\nabla\Phi|^2 d^2r. \tag{1}$$

For definiteness, we consider the case of a superfluid film, in which the field $\Phi(\mathbf{r})$ has the meaning of the velocity potential $\mathbf{v}=(1/m)\nabla\Phi$ (we set $\hbar=1$), and $K_0=n_0/2mT$, where m is the mass of a particle and n_0 is the "bare" superfluid number density obtained by averaging out microscopic fluctuations up to some mesoscopic scale l_0. Hence, $n_0\equiv n_0(l_0)$. The field Φ is then split

$$\Phi = \Phi_0 + \varphi \tag{2}$$

into a singular part Φ_0, containing all the topological defects, and a regular part φ.

By definition, Φ_0 satisfies the nonzero velocity circulation condition

$$\oint_{\mathcal{C}_j} \nabla\,\Phi_0(\mathbf{r})d\mathbf{r} = 2\pi l_j, \tag{3}$$

where $\mathcal{C}_j$ is a contour enclosing only the jth defect and l_j are integers, while $\nabla\varphi$ is circulation-free. The next crucial step is to require[2]

$$\Delta\Phi_0(\mathbf{r}) = 0 \tag{4}$$

(except for the isolated points of defects). The standard motivation of Eq. (4) is that it guarantees that Φ_0 minimizes the action when $\varphi\equiv 0$. The definitions of Φ_0 and φ thus become unambiguous and, most importantly, the action takes the form of two independent terms

$$A[\Phi] = A[\Phi_0] + A[\varphi]. \tag{5}$$

At this point, one conjectures that Φ_0 and φ correspond to vortices and phonons (spin waves, etc.), respectively. This identification, which might seem to be quite natural—or at least merely terminological and mathematically irrelevant—is not that innocent. If the two fields are not canonical vortices and phonons, then one faces a problem of *justifying* writing the partition function in the form[2]

$$Z \propto \int \exp\{-A[\varphi]\}\mathcal{D}\varphi \int \exp\{-A[\Phi_0]\}\prod_{j=1}^{N} d^2r_j, \tag{6}$$

where $\mathbf{r}_j$ is the position of the jth defect and N is the number of defects. This expression should also include the Jacobian of the transformation from canonical variables. Remarkable agreement between the Kosterlitz-Thouless theory and experimental data suggests that the Jacobian is unimportant, but without explicitly demonstrating this fact the theory is incomplete.

Apart from Jacobian, there is also an issue of peculiar "collective" behavior of formally independent fields Φ_0 and

φ. Asymptotic long-range phase correlations in a superfluid are due to phonons. The corresponding action in terms of the genuine phonon field $\tilde{\varphi}$ is

$$A_{\tilde{\varphi}} = \frac{n_s}{2mT} \int |\nabla \tilde{\varphi}|^2 d^2 r, \tag{7}$$

with n_s the macroscopic superfluid density. Would φ stand for phonons, we were to identify its long-wave harmonics with $\tilde{\varphi}$. This, however, would imply $n_0(l_0)=n_s$, which is definitely not the case since $\Phi_0 \neq 0$ at the length scale l_0. This paradox can be formulated as an observation that it is impossible to renormalize the sound velocity by vortex pairs without the *phonon-vortex coupling*. The only logical solution is then that φ is *not* a phonon field.

Another paradoxical circumstance is associated with interpreting Φ_0 as a *purely* vortex field. In a two-dimensional (2D) superfluid, all vortices are bound in microscopic pairs and one would not expect them to be *directly* observable in long-range correlation properties. The only physical way for vortex pairs to manifest themselves at the macroscopic scale is to renormalize the superfluid density. However, the requirement (4) implies that vortex pairs do contribute to the long-range correlations. The way they do it reveals a conspiracy between Φ_0 and φ.[5] Due to statistical independence of the fields Φ_0 and φ, the one-particle density matrix at large distances

$$\rho(\mathbf{r}) \propto \langle \exp[i\Phi(\mathbf{r}) - i\Phi(0)] \rangle \tag{8}$$

factorizes: $\rho(\mathbf{r}) \propto \Gamma_{\Phi_0}(\mathbf{r})\Gamma_{\varphi}(\mathbf{r})$, where

$$\Gamma_{\Phi_0}(\mathbf{r}) = \langle \exp[i\Phi_0(\mathbf{r}) - i\Phi_0(0)] \rangle, \tag{9}$$

$$\Gamma_{\varphi}(\mathbf{r}) = \langle \exp[i\varphi(\mathbf{r}) - i\varphi(0)] \rangle. \tag{10}$$

Remarkably, the independent correlation functions Γ_{Φ_0} and Γ_{φ} make no physical sense separately, since they both depend on the bare superfluid density n_0, but when the two are combined in $\rho(\mathbf{r})$, the parameter n_0 drops out, and the density matrix decays with the proper exponent $mT/2\pi n_s$.[5]

A rational explanation of this "secret agreement" between Φ_0 and φ is that being mathematically independent, the two fields are deeply connected physically. The above-mentioned structure of the correlation function even suggests a qualitative form of the connection: The long-wave part of the vortex-pair field Φ_0 actually *belongs to phonons, not vortices*.

In what follows, we trace the model (1) back to its dynamical Hamiltonian form and derive the canonical parametrization of vortices and phonons from that starting point. In doing so, we utilize the formalism recently developed by two of us,[16] from which it is directly seen that the positions of vortices $\{\mathbf{r}_j\}$ and the field φ are canonical variables *only* in the limiting cases of incompressible fluid ($\varphi \equiv 0$) and vortex-free environment ($\Phi_0 \equiv 0$), respectively. An explicit transform from $\{\mathbf{r}_j\}$ and $\varphi(\mathbf{r})$ to the canonical variables justifies that the deviation of the Jacobian from unity is irrelevant in the context of the KT theory. Our analysis allows us to reformulate KT theory in terms of canonical variables: vortex pairs and genuine phonons, coupled to each other in the most intuitive way: Vortex pairs interact with the long-wave fluctuations of the velocity field precisely the same way they interact with a homogeneous velocity field. This interaction naturally accounts for the renormalization of the long-wavelength-phonon stiffness and leads to the coarse-grained effective action in the form of Eq. (7). In complete agreement with physical understanding of vortex pairs as essentially local objects, we demonstrate that the far-field of $\Phi_0(\mathbf{r})$ belongs to phonons. Correspondingly, the long-range decay of phase correlations is governed by the statistics of long-wavelength phonons only, i.e., by the effective action (7).

Putting aside the issue of the Jacobian and *pior* to the discussion of the dynamic model, a purely statistical insight into the problem can be obtained by constructing an alternative to (Φ_0,φ) set of variables. [For simplicity, below we deal with only one vortex-antivortex pair; the generalization to finite (but small) density of pairs is straightforward.] Consider a vortex pair of separation $\mathbf{R}=\mathbf{r}_1-\mathbf{r}_2$ located at the point $\mathbf{r}_p=(\mathbf{r}_1+\mathbf{r}_2)/2$, where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the positions of the vortices with $l_1=1$ and $l_2=-1$, respectively. Introduce an auxiliary field $\varphi_0(\mathbf{r})$ such that it approaches $\Phi_0(\mathbf{r})$ when $|\mathbf{r}-\mathbf{r}_p| \gg R$, and, in contrast to $\Phi_0(\mathbf{r})$, is regular at all distances. This definition fixes the dipole moment of the new field

$$\int \mathbf{r}\Delta\varphi_0(\mathbf{r}) d^2 r = 2\pi(\mathbf{R}\times\hat{z}), \tag{11}$$

where $\hat{z}$ is a unit vector along the z axis. Make a transformation

$$\varphi(\mathbf{r}) = \tilde{\varphi}(\mathbf{r}) - \varphi_0(\mathbf{r}), \tag{12}$$

which just shifts the field φ by a regular $(\mathbf{r}_p,\mathbf{R})$-dependent field φ_0, and thus does not change the configurational volume: $\mathcal{D}\varphi=\mathcal{D}\tilde{\varphi}$. After this transformation, the long-range behavior of the density matrix is completely described in terms of the filed $\tilde{\varphi}$

$$\rho(\mathbf{r}) \propto \langle \exp[i\tilde{\varphi}(\mathbf{r}) - i\tilde{\varphi}(0)] \rangle. \tag{13}$$

This simplification comes at a price: The vortex pair now couples to $\tilde{\varphi}$. The structure of the interaction term between the pair and the long-wave harmonics of the field $\tilde{\varphi}$ (such that $\lambda \gg R$, where λ is the characteristic wavelength) is most transparent. It reads

$$A_{\mathrm{int}} = \frac{2\pi n_0}{mT}(\mathbf{R}\times\hat{z})\,\nabla\,\tilde{\varphi}\big|_{\mathbf{r}_p}, \tag{14}$$

i.e., the vortex pair interacts with the long-wave part of $\tilde{\varphi}$ exactly the same way it would interact with a homogeneous velocity flow $(1/m)\nabla\tilde{\varphi}|_{\mathbf{r}_p}$. One does not have to take this interaction into account explicitly in the KT renormalization group treatment, since its only relevant effect is to replace n_0 with n_s for phonons. [The effect of phonons on the statistics of vortex pairs is negligibly small in the limit of $R\to\infty$, as is clear from a direct estimate, see also below.] There is little doubt at this point that $\tilde{\varphi}$ corresponds to genuine phonons and one just needs to formally demonstrate this fact.

We start with Popov's hydrodynamic Lagrangian,[17]

$$L = \int d^2r[-n_0\dot{\Phi}_0 - \eta\dot{\varphi} - \eta\dot{\Phi}_0] - H, \tag{15}$$

$$H = \int d^2r\left[\frac{n_0}{2m}|\nabla\varphi|^2 + \frac{1}{2\varkappa}\eta^2 + \frac{n_0}{2m}|\nabla\Phi_0|^2 + n_0\mathbf{v}_0\cdot\nabla\Phi_0\right]. \tag{16}$$

Here, the energy functional H has been expanded to the leading order with respect to small density fluctuations $\eta \ll n_0$, Φ_0 and φ are defined by Eqs. (3) and (4), $\mathbf{v}_0$ is the velocity of a global flow, and $\varkappa$ is the compressibility. The typical vortex core size $\sim a_0 = \sqrt{\varkappa/n_0 m}$ is much smaller than any other physical length scale.

If the term $\int d^2r\eta\dot{\Phi}_0 \equiv T$ were absent, η and φ would be the canonical conjugate phonon variables, while

$$\int d^2rn_0\dot{\Phi}_0 = -2\pi n_0\sum_j l_j y_j \dot{x}_j, \tag{17}$$

where $(x_j, y_j) \equiv \mathbf{r}_j$, would imply that x_j and y_j are the canonical conjugate vortex variables. However, T is linear in the time derivatives of x_j and y_j and also contains η making the set of variables $\{\eta,\varphi\}$, $\{\mathbf{r}_j\}$ not canonical, and meaning that H in these variables is not a Hamiltonian.

We are interested here only in the KT theory for the superfluid phase in the vicinity of the transition, including the critical point, where the concentration of vortex pairs of size $\sim R$ is much smaller than R^{-2} as $R\to\infty$. Correspondingly, at a phonon wavelength λ only pairs with $R \ll \lambda$ contribute to the renormalization of the sound velocity. This allows us to use the small parameter

$$R/\lambda \ll 1 \tag{18}$$

for deriving canonical variables in the form of a regular perturbative expansion starting from the zeroth approximation $\{\eta,\varphi,\mathbf{r}_j\}$.[16]

It is straightforward to show that

$$T = \sum_j 2\pi l_j[\hat{\mathbf{z}} \times \nabla Q(\mathbf{r}_j)]\dot{\mathbf{r}}_j, \tag{19}$$

where $Q(\mathbf{r})$ is defined by $\Delta Q(\mathbf{r}) = \eta(\mathbf{r})$. We first switch to the Fourier representation of $\{\eta,\varphi\}$

$$\eta(\mathbf{r}) = \sum_{\mathbf{q}} \sqrt{\omega_{\mathbf{q}}\varkappa/2V}[e^{i\mathbf{qr}}c_{\mathbf{q}} + e^{-i\mathbf{qr}}c^*_{\mathbf{q}}],$$

$$\varphi(\mathbf{r}) = -i\sum_{\mathbf{q}} \sqrt{1/2V\omega_{\mathbf{q}}\varkappa}[e^{i\mathbf{qr}}c_{\mathbf{q}} - e^{-i\mathbf{qr}}c^*_{\mathbf{q}}], \tag{20}$$

where $\omega_{\mathbf{q}} = (\sqrt{n_0/\varkappa m})q$ and $\{c_{\mathbf{q}}, c^*_{\mathbf{q}}\}$ are resembling (and to the zeroth approximation coincide with) the classical-field counterparts of phonon creation and annihilation operators, and V is the system volume. Let the vortex $(l_1=1)$ and the antivortex $(l_2=-1)$ in a pair have coordinates $\mathbf{r}_1 = \mathbf{r}_p + \mathbf{R}/2$ and $\mathbf{r}_2 = \mathbf{r}_p - \mathbf{R}/2$, respectively. Next, we expand $Q(\mathbf{r}_j)$ in T into series with respect to $qR \ll 1$. The resulting terms are eliminated by iteratively correcting the variables $\{\mathbf{r}_j\}$, $\{c_{\mathbf{q}}, c^*_{\mathbf{q}}\}$ as described in Ref. 16, so that the Lagrangian takes on the canonical form

$$L = \sum_{\mathbf{q}} i\dot{\tilde{c}}_{\mathbf{q}}\tilde{c}^*_{\mathbf{q}} + 2\pi n_0 \sum_j l_j \tilde{y}_j \dot{\tilde{x}}_j - H\{\tilde{\mathbf{r}}_j, \tilde{c}_{\mathbf{q}}, \tilde{c}^*_{\mathbf{q}}\}, \tag{21}$$

where $\tilde{\mathbf{r}}_j = (\tilde{x}_j, \tilde{y}_j)$ and $\tilde{c}_{\mathbf{q}}$, $\tilde{c}^*_{\mathbf{q}}$ are the Hamiltonian variables. For our purposes we shall need only the leading correction, which does not change the vortex variables

$$\mathbf{r}_j = \tilde{\mathbf{r}}_j, \tag{22}$$

and for the phonon variables, yields

$$c_{\mathbf{q}} = \tilde{c}_{\mathbf{q}} + 2\pi\sqrt{\frac{n_0 a_0 q}{2V_2}}\frac{[q_x\tilde{R}_y - q_y\tilde{R}_x]}{q^2}e^{i\mathbf{q}\tilde{\mathbf{r}}_p}, \tag{23}$$

where an equivalent set of vortex variables $\tilde{\mathbf{R}} = \tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_2$, $\tilde{\mathbf{r}}_p = (\tilde{\mathbf{r}}_1 + \tilde{\mathbf{r}}_2)/2$, is used. The Jacobian of the transformations (22) and (23) equals unity. If higher-order (in $\eta/n_0 \ll 1$ and $qR \ll 1$) terms are included in Eqs. (22) and (23), the deviation of the Jacobian from unity is of the order of $(\eta/n_0)(qR)$. From now on we omit the tildes over the vortex canonical variables in view of Eq. (22).

The canonical phonon fields, $\tilde{\eta}$, $\tilde{\varphi}$, are defined analogously to Eq. (20), with $\{\tilde{c}_{\mathbf{q}}, \tilde{c}^*_{\mathbf{q}}\}$ replacing $\{c_{\mathbf{q}}, c^*_{\mathbf{q}}\}$. After substituting Eq. (23) for $c_{\mathbf{q}}$ in Eq. (20) and taking the sum over $\mathbf{q}$ the original variable φ is expressed in terms of the canonical variables as

$$\varphi(\mathbf{r}) = \tilde{\varphi}(\mathbf{r}) - \frac{[(\mathbf{r}-\mathbf{r}_p)_y R_x - (\mathbf{r}-\mathbf{r}_p)_x R_y]}{|\mathbf{r}-\mathbf{r}_p|^2}. \tag{24}$$

Now we note that at large distances from the vortex pair $|\mathbf{r}-\mathbf{r}_p| \gg R$, the field $\Phi_0(\mathbf{r})$ is given by[5]

$$\Phi_0(\mathbf{r}) = \frac{[(\mathbf{r}-\mathbf{r}_p)_y R_x - (\mathbf{r}-\mathbf{r}_p)_x R_y]}{|\mathbf{r}-\mathbf{r}_p|^2}. \tag{25}$$

Along with Eq. (24), this implies that sufficiently far from $\mathbf{r_p}$, $\Phi_0(\mathbf{r})$ does not belong to the vortex-anti-vortex pair at all, but is actually a part of the phonon field $\tilde{\varphi}$.

After a standard algebra, the Hamiltonian assumes the form

$$H = H_{\mathrm{v}} + H_{\mathrm{ph}} + H_{\mathrm{int1}} + H_{\mathrm{int2}},$$

$$H_{\mathrm{v}} = \frac{2\pi n_0}{m}\ln(R/l_0) + 2E_c,$$

$$H_{\mathrm{ph}} = \int d^2r\left[\frac{n_0}{2m}|\nabla\tilde{\varphi}|^2 + \frac{1}{2\varkappa}\tilde{\eta}^2\right],$$

$$H_{\mathrm{int1}} = 2\pi n_0(\mathbf{R}\times\hat{z})\mathbf{v}_0,$$

$$H_{\mathrm{int2}} = \frac{2\pi n_0}{m}(\mathbf{R}\times\hat{z})\nabla\tilde{\varphi}\bigg|_{\mathbf{r}_p}. \tag{26}$$

This form is almost identical to the original effective action in terms of $\mathbf{R}$ and φ of Refs. 2 and 5–7. Besides the presence of η, which is trivially integrated out in the partition function, the only distinctive feature of the Hamiltonian (26) is the term H_{int2}, which couples the vortex dipole moment $\mathbf{R}$ to the fluid velocity in the sound wave $\propto\nabla\tilde{\varphi}|_{\mathbf{r}_p}$.

Consider the thermodynamics of the system (26) near the critical point $T_c = \pi n_s / 2m$. The coupling term H_{int2} does not change the statistics of vortices, since its typical value is small, $H_{\mathrm{int2}}/T \sim qR \lesssim 1$, whereas the contribution of H_{v} diverges logarithmically. Therefore, the superfluid density $n_s = (1/mV)\partial^2 F/\partial v_{0\alpha}^2|_{\mathrm{v}_0=0}$, $\alpha = x, y$, where $F = -T \ln Z$, is given by the Kosterlitz renormalization group flow.[5] In contrast, H_{int2} is essential for the phonon statistics. Since its structure is identical to the vortex coupling to the uniform flow, averaging over $\mathbf{R}$ and $\mathbf{r}_p$ straightforwardly leads to the coarse-grained effective action for the long-wavelength phonons governed by the renormalized stiffness Eq. (7).

To summarize, we have shown that the simplicity of the parametrization (2)–(4)—the statistical independence of the fields Φ_0 and φ—comes at a price of the substantial lack of its physical meaning, apart from the inconvenience of calculating off-diagonal correlators, where direct contribution of vortex pairs has to be explicitly evaluated with the only goal to replace bare superfluid density n_0 with its renormalized value. An alternative parametrization in terms of phonon variables (or their *XY* equivalents) renders the Kosterlitz-Thouless scheme even more mathematically simple and accurate, while making it physically transparent. The vortex-phonon interaction that appears in the effective Hamiltonian does not lead to any complications, because the structure of this interaction is exactly the same as that of the interaction of vortex pairs with a homogeneous external flow and the only effect of this interaction is to ensure that *both* phonons and vortices are controlled by the renormalized superfluid density.

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