

# Markov-Chain Monte-Carlo simulations of a $p_x \pm ip_y$ superconductor

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## 1 Derivation of discretized free energy

The dimensionless Ginzburg-Landau (GL) free energy density for a two-component  $p_x \pm ip_y$  order parameter used in [1] is given by

$$\begin{aligned} \mathcal{F} = & |\nabla \times \mathbf{A}|^2 + |\mathbf{D}\eta^+|^2 + |\mathbf{D}\eta^-|^2 \\ & + (\nu + 1) \operatorname{Re} [(D_x\eta^+)^* D_x\eta^- - (D_y\eta^+)^* D_y\eta^-] \\ & + (\nu - 1) \operatorname{Im} [(D_x\eta^+)^* D_y\eta^- + (D_y\eta^+)^* D_x\eta^-] \\ & + 2|\eta^+\eta^-|^2 + \nu \operatorname{Re} ((\eta^+)^*{}^2 (\eta^-)^2) + \sum_{h=\pm} \left[ -|\eta^h|^2 + \frac{1}{2}|\eta^h|^4 \right], \end{aligned} \quad (1)$$

where  $\eta^\pm = \rho_\pm e^{i\theta^\pm}$  are the components of the superconducting order parameter. The lengths are given in terms of  $\xi = [\alpha_0(T - T_c)]^{-1/2}$ , the magnetic field  $\mathbf{B} = \nabla \times \mathbf{A}$  is given in units of  $\sqrt{2}B_C = \Phi_0/(2\pi\lambda\xi)$ . The dimensionless gauge coupling used in the covariant derivatives  $\mathbf{D} = \nabla + ig\mathbf{A}$  is used to parametrize the ratio of two length scales  $g^{-1} = \kappa = \lambda/\xi$ . On the first line of the equation, we see the Maxwell term as well as the normal kinetic terms associated with the order parameter components. The second line exhibits Andreev-Bashkin terms while the third line contains what we call mixed gradient terms (MGT) where both different components and gradients are mixed.

Note that the theory is gauge invariant under the local gauge transformation

$$\eta^h \mapsto e^{i\lambda} \eta^h \quad (2a)$$

$$\mathbf{A} \mapsto \mathbf{A} - \frac{1}{g} \nabla \lambda. \quad (2b)$$

### 1.1 London approximation

Assuming that the amplitude of the GL order parameters are constant (London approximation), such that  $\eta^h(\mathbf{r}) = \rho_h e^{i\theta^h(\mathbf{r})}$  and inserting that the components of the covariant derivative is given by  $D_\mu = \partial_\mu + igA_\mu$ , the free energy based on the density  $\mathcal{F}$  in Eq. (1) becomes

$$\begin{aligned} F^{\text{lon}} = & \int d^2r \left\{ |\nabla \times \mathbf{A}|^2 + \sum_{\mu,h} \rho_h^2 (\partial_\mu \theta^h + gA_\mu)^2 \right. \\ & + \rho_+ \rho_- (\nu + 1) \cos(\theta^+ - \theta^-) \left[ (\partial_x \theta^+ + gA_x)(\partial_x \theta^- + gA_x) - (\partial_y \theta^+ + gA_y)(\partial_y \theta^- + gA_y) \right] \\ & + \rho_+ \rho_- (\nu - 1) \sin(\theta^- - \theta^+) \left[ (\partial_x \theta^- + gA_x)(\partial_y \theta^+ + gA_y) + (\partial_y \theta^+ + gA_y)(\partial_x \theta^+ + gA_x) \right] \\ & \left. + \nu \rho_+^2 \rho_-^2 \cos 2(\theta^+ - \theta^-) \right\} + \mathcal{V} \left\{ \sum_h \left[ -\rho_h^2 + \frac{1}{2} \rho_h^4 \right] + 2\rho_+ \rho_- \right\}. \end{aligned} \quad (3)$$

In the sums in this equation,  $h \in \{\pm\}$  while  $\mu \in \{x, y\}$ .  $\mathcal{V}$  denotes the volume of the system. The terms proportional to  $\mathcal{V}$  are usually ignored, but since we will consider globally varying  $\rho_{\pm}$  in the Monte-Carlo simulation, we have included them here for completeness.

## 1.2 Lattice regularization

The discretization of the continuum models above onto a two-dimensional lattice is done through a number of mappings [2, 3, 4]. Integrals over space are mapped to a sum over lattice positions  $\mathbf{r}$  by

$$\int d^D x \mapsto a^D \sum_{\mathbf{r}}, \quad (4)$$

where  $a$  is the length between lattice sites. Since the numerical lattice has square symmetry, only one length parameter is necessary. The 6 degrees of freedom go from being continuous variables  $\eta^{\pm}, \eta^{\pm*}, \mathbf{A}$ , to begin discretized variables where the superconducting order parameter gets an associated variable at each lattice site  $\eta_{\mathbf{r}}^{\pm}, \eta_{\mathbf{r}}^{\pm*}$ , while the vector potential  $\mathbf{A}$  is discretized by link variables  $A_{\mathbf{r},\mu}$  between the lattice site at  $\mathbf{r}$  and the nearest neighbor in direction  $\hat{\mu}$ . Covariant derivatives are replaced by

$$D_{\mu}\eta^h = (\partial_{\mu} + igA_{\mu})\eta^h \mapsto a^{-1}(\eta_{\mathbf{r}+\hat{\mu}}^h e^{igaA_{\mathbf{r},\mu}} - \eta_{\mathbf{r}}^h). \quad (5)$$

Note the abuse of vector notation in  $\eta_{\mathbf{r}+\hat{\mu}}^h$  which is a shorthand for the nearest neighbor of the lattice site  $\mathbf{r}$  in the  $\hat{\mu}$  direction. In this notation, the definition of the difference operator  $\Delta_{\mu}$  becomes

$$\Delta_{\mu}A_{\mathbf{r},\nu} = A_{\mathbf{r}+\hat{\mu},\nu} - A_{\mathbf{r},\nu}. \quad (6)$$

Finally the continuous version of the Maxwell term which is responsible for the free energy of the electromagnetic field, is replaced by a sum over all plaquettes of the lattice

$$\begin{aligned} \int d^D r (\nabla \times \mathbf{A})^2 &\mapsto a^{D-2} \sum_{\mathbf{r}} (\Delta \times \mathbf{A}_{\mathbf{r}})^2 = a^{D-2} \sum_{\mathbf{r},\mu} (\epsilon_{\mu\nu\lambda} \Delta_{\nu} A_{\mathbf{r},\lambda})^2 \\ &= a^{D-2} \sum_{\mathbf{r},\mu>\nu} (\Delta_{\mu} A_{\mathbf{r},\nu} - \Delta_{\nu} A_{\mathbf{r},\mu})^2. \end{aligned} \quad (7)$$

This is the noncompact way of discretizing the vector potential, i.e.  $A_{\mathbf{r},\mu} \in (-\infty, \infty)$ . In the compact version, the link variables  $A_{\mathbf{r},\mu}$  have  $2\pi$  periodicity and generally allows topologically nontrivial excitations such as magnetic monopoles [4] for large fluctuations of the vector potential.

To ensure proper boundary conditions of the vector potential we will split it in a constant and fluctuating field such that  $\mathbf{A}_{\mathbf{r}} = \mathbf{A}_{\mathbf{r}}^0 + \mathbf{A}_{\mathbf{r}}^f$ , where  $\mathbf{A}_{\mathbf{r}}^0 = (0, 2\pi f r_x, 0)^T$ . Here  $f$  is the magnetic filling fraction while  $r_x$  is the  $x$  position of lattice site  $\mathbf{r}$ . Letting the fluctuating field  $A_{\mathbf{r}}^f$  have periodic boundary conditions hence ensures that there will be a constant external magnetic field  $\mathbf{B} = (0, 0, 2\pi f)$  penetrating the lattice [5]. The Maxwell term then is divided in three terms

$$F_A = a^{D-2} \sum_{\mathbf{r}} \left[ (\Delta \times \mathbf{A}_{\mathbf{r}}^0)^2 + (\Delta \times \mathbf{A}_{\mathbf{r}}^f)^2 + 2(\Delta \times \mathbf{A}_{\mathbf{r}}^0) \cdot (\Delta \times \mathbf{A}_{\mathbf{r}}^f) \right], \quad (8)$$

where the first one is constant and hence it can be neglected. Since the model under consideration is of a  $2D$  lattice, the link variables  $A_{\mathbf{r},z}$  out of the plane are neglected as well as any difference in the  $z$ -direction  $\Delta_z A_{\mathbf{r},\mu}$ . This simplifies the expression for  $\Delta \times \mathbf{A}_{\mathbf{r}}$  in Eq. (7) to only the  $z$ -component  $\Delta \times \mathbf{A}_{\mathbf{r}} = \hat{z}(\Delta_x A_{\mathbf{r},y} - \Delta_y A_{\mathbf{r},x})$ . Denoting the  $z$ -component of the discretized curl of the fluctuating field

$$A_{\square,\mathbf{r}}^f \equiv \Delta_x A_{\mathbf{r},y}^f - \Delta_y A_{\mathbf{r},x}^f = A_{\mathbf{r},x}^f + A_{\mathbf{r}+\hat{x},y}^f - A_{\mathbf{r}+\hat{y},x}^f - A_{\mathbf{r},y}^f, \quad (9)$$

this can be interpreted as the sum of the fluctuating vector potential over the plaquette  $\square$  at the lattice site  $\mathbf{r}$ . With this definition, the Maxwell term in Eq. (8) can be written

$$\begin{aligned} F_A &= \sum_{\mathbf{r}} \left\{ (A_{\square, \mathbf{r}}^f)^2 + 2(\Delta_x A_{\mathbf{r}, y}^0 - \Delta_y A_{\mathbf{r}, x}^0) A_{\square, \mathbf{r}}^f \right\} \\ &= \sum_{\mathbf{r}} (A_{\square, \mathbf{r}}^f)^2 + 2 \cdot 2\pi f a \sum_{\mathbf{r}} A_{\square, \mathbf{r}}^f = \sum_{\mathbf{r}} (A_{\square, \mathbf{r}}^f)^2. \end{aligned} \quad (10)$$

In the second line we have evaluated the specific expression for the constant vector potential. In the third, we realize that the sum over  $A_{\square, \mathbf{r}}^f$  vanishes by shifting lattice indices.

Applying this procedure to the free energy density in Eq. (1) yields the free energy  $F$ , which we divide into terms

$$F^{\text{disc}} = F_K + F_{\text{MGT}} + F_V + F_A. \quad (11)$$

The potential term is given by

$$F_V = a^2 \sum_{\mathbf{r}} \left\{ \sum_h \left[ -|\eta_{\mathbf{r}}^h|^2 + \frac{1}{2} |\eta_{\mathbf{r}}^h|^4 \right] + 2|\eta_{\mathbf{r}}^+ \eta_{\mathbf{r}}^-|^2 + \nu \text{Re} [(\eta_{\mathbf{r}}^+)^*{}^2 (\eta_{\mathbf{r}}^-)^2] \right\}, \quad (12)$$

while the Maxwell term  $F_A$  is given by the expression to the right in Eq. (10). The variables on the numerical lattice is assumed to be periodic - when e.g.  $\eta_{\mathbf{r}+\hat{\mu}}^h$  is evaluated at a lattice site  $\mathbf{r}+\hat{\mu}$  outside the lattice, we wrap around. Utilizing this assumption, the regularized representation of the normal kinetic terms without mixed gradients becomes

$$F_K = \sum_{\mathbf{r}, \mu, h} \left\{ 2|\eta_{\mathbf{r}}^h|^2 - [(\eta_{\mathbf{r}+\hat{\mu}}^h)^* \eta_{\mathbf{r}}^h e^{-igaA_{\mathbf{r}, \mu}} + \text{c.c.}] \right\}. \quad (13)$$

The mixed gradient terms of  $\mathcal{F}$  in Eq. (1) forms the regularized free energy

$$\begin{aligned} F_{\text{MGT}} &= \sum_{\mathbf{r}} \left\{ (\nu + 1) \text{Re} \left[ \eta_{\mathbf{r}}^- * (\eta_{\mathbf{r}+\hat{y}}^+ e^{igaA_{\mathbf{r}, y}} - \eta_{\mathbf{r}+\hat{x}}^+ e^{igaA_{\mathbf{r}, x}}) + \eta_{\mathbf{r}}^+ (\eta_{\mathbf{r}+\hat{y}}^- e^{-igaA_{\mathbf{r}, y}} - \eta_{\mathbf{r}+\hat{x}}^- e^{-igaA_{\mathbf{r}, x}}) \right] \right. \\ &\quad + (\nu - 1) \text{Im} \left[ (\eta_{\mathbf{r}+\hat{y}}^+ * \eta_{\mathbf{r}+\hat{x}}^- - \eta_{\mathbf{r}+\hat{y}}^- * \eta_{\mathbf{r}+\hat{x}}^+) e^{iga(A_{\mathbf{r}, x} - A_{\mathbf{r}, y})} + 2\eta_{\mathbf{r}}^+ * \eta_{\mathbf{r}}^- \right. \\ &\quad \left. \left. + (\eta_{\mathbf{r}}^- * \eta_{\mathbf{r}+\hat{x}}^+ - \eta_{\mathbf{r}}^+ * \eta_{\mathbf{r}+\hat{x}}^-) e^{igaA_{\mathbf{r}, x}} + (\eta_{\mathbf{r}+\hat{y}}^- * \eta_{\mathbf{r}}^+ - \eta_{\mathbf{r}+\hat{y}}^+ * \eta_{\mathbf{r}}^-) e^{-igaA_{\mathbf{r}, y}} \right] \right\}. \end{aligned} \quad (14)$$

The regularized free energy is invariant under the gauge-transformation

$$\eta_{\mathbf{r}}^h \mapsto e^{i\lambda_{\mathbf{r}}} \eta_{\mathbf{r}}^h \quad (15a)$$

$$A_{\mathbf{r}, \mu} \mapsto A_{\mathbf{r}, \mu} - \frac{\Delta_{\mu} \lambda_{\mathbf{r}}}{ga}. \quad (15b)$$

### 1.3 Lattice regularization + London approximation

Similarly to what we did for Eq. (3), we assume that the amplitude of the components of the order-parameter are constant such that  $\eta_{\mathbf{r}}^h = \rho_h e^{i\theta_{\mathbf{r}}^h}$ . Inserting this assumption into the different terms of the free energy  $F$  in Eq. (11) yields the normal kinetic free energy

$$F_K^{\text{lon}} = 2 \sum_{\mathbf{r}, \mu, h} \rho_h^2 \left\{ 1 - \cos(\Delta_{\mu} \theta_{\mathbf{r}}^h + gaA_{\mathbf{r}, \mu}) \right\}, \quad (16)$$

the free energy given by the potential terms

$$F_V^{\text{lon}} = a^2 \mathcal{N} \left\{ \sum_h \left[ -\rho_h^2 + \frac{1}{2} \rho_h^4 \right] + (2 - \nu) \rho_+^2 \rho_-^2 \right\} + 2\rho_+^2 \rho_-^2 a^2 \nu \sum_{\mathbf{r}} \cos^2(\theta_{\mathbf{r}}^+ - \theta_{\mathbf{r}}^-), \quad (17)$$

as well as the MGT free energy

$$\begin{aligned}
F_{\text{MGT}}^{\text{lon}} = & \rho_+ \rho_- \sum_{\mathbf{r}} \left\{ (\nu + 1) \left[ \cos(\theta_{\mathbf{r}+\hat{y}}^+ - \theta_{\mathbf{r}}^- + gaA_{\mathbf{r},y}) - \cos(\theta_{\mathbf{r}+\hat{x}}^+ - \theta_{\mathbf{r}}^- + gaA_{\mathbf{r},x}) \right. \right. \\
& \left. \left. + \cos(\theta_{\mathbf{r}+\hat{y}}^- - \theta_{\mathbf{r}}^+ + gaA_{\mathbf{r},y}) - \cos(\theta_{\mathbf{r}+\hat{x}}^- - \theta_{\mathbf{r}}^+ + gaA_{\mathbf{r},x}) \right] \right. \\
& \left. + (\nu - 1) \left[ \sin(\theta_{\mathbf{r}+\hat{x}}^- - \theta_{\mathbf{r}+\hat{y}}^+ + ga(A_{\mathbf{r},x} - A_{\mathbf{r},y})) + \sin(\theta_{\mathbf{r}+\hat{y}}^- - \theta_{\mathbf{r}+\hat{x}}^+ + ga(A_{\mathbf{r},y} - A_{\mathbf{r},x})) \right. \right. \\
& \left. \left. + 2 \sin(\theta_{\mathbf{r}}^- - \theta_{\mathbf{r}}^+) + \sin(\theta_{\mathbf{r}+\hat{x}}^+ - \theta_{\mathbf{r}}^- + gaA_{\mathbf{r},x}) - \sin(\theta_{\mathbf{r}+\hat{x}}^- - \theta_{\mathbf{r}}^+ + gaA_{\mathbf{r},x}) \right. \right. \\
& \left. \left. - \sin(\theta_{\mathbf{r}+\hat{y}}^- - \theta_{\mathbf{r}}^+ + gaA_{\mathbf{r},y}) + \sin(\theta_{\mathbf{r}+\hat{y}}^+ - \theta_{\mathbf{r}}^- + gaA_{\mathbf{r},y}) \right] \right\}.
\end{aligned} \tag{18}$$

The big question is what justification this assumption is based on. In [4] they also have a two-component  $p$ -wave order parameter, but they rather assume that  $\sum_h |\eta^h|^2 = \text{const.}$  in what they call the London-approximation. Choosing units such that this constant is 1, then  $\eta^h$  is a complex projective field.

#### 1.4 London approximation by a $\mathbb{CP}^1$ -field

Instead of fixing the amplitude of each field as in the London approximation, a less strict approximation is to say that

$$|\eta_{\mathbf{r}}^+|^2 + |\eta_{\mathbf{r}}^-|^2 = \gamma^2, \tag{19}$$

for a constant  $\gamma > 0$ , i.e. the sum of squares of the amplitudes of the components together is constant. This makes it possible that condensate from one component can flow into the other and vice versa. Defining two new fields

$$z_{\mathbf{r}}^h \equiv \frac{1}{\gamma} \eta_{\mathbf{r}}^h = \frac{1}{\gamma} \rho_{\mathbf{r}}^h e^{i\theta_{\mathbf{r}}^h} \equiv u_{\mathbf{r}}^h e^{i\theta_{\mathbf{r}}^h}, \tag{20}$$

the constraint on  $\eta_{\mathbf{r}}^h$  in Eq. (19) becomes the  $\mathbb{CP}^1$  constraint

$$|z_{\mathbf{r}}^+|^2 + |z_{\mathbf{r}}^-|^2 = 1 \tag{21}$$

when written in terms of the new fields. This constraint reduces the real degrees of freedom in the fields from 4 to 3. Choosing the amplitude  $u_{\mathbf{r}}^+$  as the free degree of freedom, the constraint implies that  $u_{\mathbf{r}}^- = \sqrt{1 - (u_{\mathbf{r}}^+)^2}$ . Rewriting the free energy in Eq. (11) in terms of these new degrees of freedom and ignoring constant terms yields

$$\begin{aligned}
F_K = & \gamma^2 \sum_{\mathbf{r}, \mu, h} \left[ 2|u_{\mathbf{r}}^h|^2 - \left( u_{\mathbf{r}+\hat{\mu}}^h u_{\mathbf{r}}^h e^{-i(\theta_{\mathbf{r}+\hat{\mu}}^h - \theta_{\mathbf{r}}^h + gaA_{\mathbf{r},\mu})} + \text{c.c.} \right) \right] \\
= & 2\gamma^2 \sum_{\mathbf{r}, \mu} -2\gamma^2 \sum_{\mathbf{r}, \mu, h} u_{\mathbf{r}+\hat{\mu}}^h u_{\mathbf{r}}^h \cos(\theta_{\mathbf{r}+\hat{\mu}}^h - \theta_{\mathbf{r}}^h + gaA_{\mathbf{r},\mu}) \\
\sim & -2\gamma^2 \sum_{\mathbf{r}, \mu, h} u_{\mathbf{r}+\hat{\mu}}^h u_{\mathbf{r}}^h \cos(\theta_{\mathbf{r}+\hat{\mu}}^h - \theta_{\mathbf{r}}^h + gaA_{\mathbf{r},\mu}),
\end{aligned} \tag{22}$$

for the normal kinetic term in Eq. (13),

$$\begin{aligned}
F_V = & a^2 \sum_{\mathbf{r}} \left\{ \sum_h \left[ -\gamma^2 u_{\mathbf{r}}^{h2} + \frac{\gamma^4}{2} u_{\mathbf{r}}^{h4} \right] + 2\gamma^4 (u_{\mathbf{r}}^+ u_{\mathbf{r}}^-)^2 + \nu \gamma^4 (u_{\mathbf{r}}^+ u_{\mathbf{r}}^-)^2 \text{Re} e^{2i(\theta_{\mathbf{r}}^- - \theta_{\mathbf{r}}^+)} \right\} \\
= & a^2 \sum_{\mathbf{r}} \left\{ -\gamma^2 + \frac{1}{2} \gamma^4 (u_{\mathbf{r}}^{+4} + 1 - 2u_{\mathbf{r}}^{+2} + u_{\mathbf{r}}^{+4}) + \gamma^4 u_{\mathbf{r}}^{+2} u_{\mathbf{r}}^{-2} \left[ 2 + \nu \cos 2(\theta_{\mathbf{r}}^+ - \theta_{\mathbf{r}}^-) \right] \right\} \\
= & a^2 (-\gamma^2 + \gamma^4/2) \sum_{\mathbf{r}} + a^2 \sum_{\mathbf{r}} \left\{ \gamma^4 u_{\mathbf{r}}^{+2} (u_{\mathbf{r}}^{+2} - 1) + \gamma^4 u_{\mathbf{r}}^{+2} u_{\mathbf{r}}^{-2} \left[ 2 + \nu \cos 2(\theta_{\mathbf{r}}^+ - \theta_{\mathbf{r}}^-) \right] \right\} \\
\sim & a^2 \gamma^4 \sum_{\mathbf{r}} u_{\mathbf{r}}^{+2} u_{\mathbf{r}}^{-2} [1 + \nu \cos 2(\theta_{\mathbf{r}}^+ - \theta_{\mathbf{r}}^-)]
\end{aligned} \tag{23}$$

for the potential term in Eq. (12) and

$$\begin{aligned}
F_{\text{MGT}} = \gamma^2 \sum_{\mathbf{r}} \Big\{ & (\nu + 1) \left[ u_{\mathbf{r}}^- u_{\mathbf{r}+\hat{y}}^+ \cos(\theta_{\mathbf{r}+\hat{y}}^+ - \theta_{\mathbf{r}}^- + agA_{\mathbf{r},y}) + u_{\mathbf{r}}^+ u_{\mathbf{r}+\hat{y}}^- \cos(\theta_{\mathbf{r}+\hat{y}}^- - \theta_{\mathbf{r}}^+ + agA_{\mathbf{r},y}) \right. \\
& - \left( u_{\mathbf{r}}^- u_{\mathbf{r}+\hat{x}}^+ \cos(\theta_{\mathbf{r}+\hat{x}}^+ - \theta_{\mathbf{r}}^- + agA_{\mathbf{r},x}) + u_{\mathbf{r}}^+ u_{\mathbf{r}+\hat{x}}^- \cos(\theta_{\mathbf{r}+\hat{x}}^- - \theta_{\mathbf{r}}^+ + agA_{\mathbf{r},x}) \right) \Big] \\
& + (\nu - 1) \left[ u_{\mathbf{r}+\hat{y}}^+ u_{\mathbf{r}+\hat{x}}^- \sin(\theta_{\mathbf{r}+\hat{x}}^- - \theta_{\mathbf{r}+\hat{y}}^+ + ga(A_{\mathbf{r},x} - A_{\mathbf{r},y})) \right. \\
& - u_{\mathbf{r}+\hat{y}}^- u_{\mathbf{r}+\hat{x}}^+ \sin(\theta_{\mathbf{r}+\hat{x}}^+ - \theta_{\mathbf{r}+\hat{y}}^- + ga(A_{\mathbf{r},x} - A_{\mathbf{r},y})) + 2u_{\mathbf{r}}^+ u_{\mathbf{r}}^- \sin(\theta_{\mathbf{r}}^- - \theta_{\mathbf{r}}^+) \\
& + u_{\mathbf{r}}^- u_{\mathbf{r}+\hat{x}}^+ \sin(\theta_{\mathbf{r}+\hat{x}}^+ - \theta_{\mathbf{r}}^- + gaA_{\mathbf{r},x}) - u_{\mathbf{r}}^+ u_{\mathbf{r}+\hat{x}}^- \sin(\theta_{\mathbf{r}+\hat{x}}^- - \theta_{\mathbf{r}}^+ + gaA_{\mathbf{r},x}) \\
& \left. \left. - \left( u_{\mathbf{r}}^- u_{\mathbf{r}+\hat{y}}^+ \sin(\theta_{\mathbf{r}+\hat{y}}^+ - \theta_{\mathbf{r}}^- + gaA_{\mathbf{r},y}) - u_{\mathbf{r}}^+ u_{\mathbf{r}+\hat{y}}^- \sin(\theta_{\mathbf{r}+\hat{y}}^- - \theta_{\mathbf{r}}^+ + gaA_{\mathbf{r},y}) \right) \right] \right\}, \tag{24}
\end{aligned}$$

for the mixed gradient terms in Eq. (14). The Maxwell term is unchanged from its form in Eq. (10).

## 2 Observables

### 2.1 Local vorticity

We are interested in investigating the vortex structure of the phase  $\theta^h(\mathbf{r})$  of the superconducting condensate components. A vortex of this kind can be imagined if we picture  $\theta^h$  as the angle of a vector in the plane. Having a vector at each position in a flat plane, we now follow the vector as we walk in a circle in the plane. If the vector makes a single rotation, like the hand in a watch, as we go around the circle clockwise, we have a vortex with a single topological charge [6]. This procedure of going in a closed orbit around the vortex and measuring how the vector rotates as we move in the trajectory can be formalized by integrating the gradient  $\nabla\theta^h$  around the path. Since we end up where we started, the vector must have rotated an integer number of times ( $n \in \mathbb{Z}$ ), and thus we get

$$\oint_{\mathcal{C}} \nabla\theta^h \cdot d\mathbf{l} = 2\pi n \tag{25}$$

The integer  $n$  is then the topological charge of the vortex [7], it is a winding number of the phase as it counts the number of times the phase winds around  $2\pi$ . It is also related to the number of quanta of magnetic flux the vortex admits — *that which we call a rose by any other name would smell as sweet*.

Let's say that all vortices in our sample has a single charge, i.e.  $n = 1$  for all vortices. The number of vortices  $N_{\text{vor}}$  can then be counted by extending the closed path  $\mathcal{C}$  to encompass our entire sample and dividing by  $2\pi$ . By Stoke's theorem then

$$N_{\text{vor}} = \frac{1}{2\pi} \iint_{\mathcal{S}} (\nabla \times \nabla\theta^h) \cdot \hat{n} \, d^2r, \tag{26}$$

where  $\mathcal{S}$  is the surface enclosed by  $\mathcal{C}$  and  $\hat{n}$  is a unit vector pointing out from this surface according to the right hand rule. From this it is natural to define the local vorticity vector as

$$\hat{\mathbf{n}}^{(h)}(\mathbf{r}) \equiv \frac{1}{2\pi} \nabla \times \nabla\theta^h(\mathbf{r}). \tag{27}$$

Normally  $\nabla \times \nabla f(\mathbf{r}) = \mathbf{0}$  for an analytic function  $f(\mathbf{r})$  so you might be worried that  $\mathbf{n}^h = \mathbf{0}$ , but fear not:  $\theta^h$  is only defined up to modulo  $2\pi$  and is thus not analytic. A vortex is in this sense a singularity in  $\nabla\theta^h$ .

There is however a problem with Eq. (27) for using it as an observable in our system, which is that by a local gauge transformation we can make it take on any value we choose. This can be

amended by using the vector potential  $\mathbf{A}$  to redefine  $\tilde{\mathbf{n}}^{(h)}$  into the gauge invariant local vorticity [5]

$$\mathbf{n}^{(h)}(\mathbf{r}) \equiv \frac{1}{2\pi} \nabla \times [\nabla \theta^h + g\mathbf{A}]. \quad (28)$$

## 2.2 Lattice regularization of $\mathbf{n}^{(h)}(\mathbf{r})$

We have so far in this section worked in the continuum, however when doing Monte-Carlo  $\theta^h(\mathbf{r}) \mapsto \theta_{\mathbf{r}}^h$  and thus only takes on discrete values. We therefore need to lattice regularize our observable  $\mathbf{n}^{(h)}$ . When regularizing the Maxwell term in the free energy in Eq. (7) we used the general procedure

$$\partial_\mu f(\mathbf{r}) \mapsto \frac{1}{a} \Delta_\mu f_{\mathbf{r}} \quad (29)$$

for a general field  $f(\mathbf{r})$ . Using this regularization and remembering that  $\theta^h(\mathbf{r})$  is a phase field such that  $(\nabla \theta^h + g\mathbf{A})$  has to be interpreted modulo  $2\pi$ , the lattice regularization of  $n_z^{(h)}(\mathbf{r})$  becomes

$$\begin{aligned} n_z^{(h)}(\mathbf{r}) \mapsto \frac{1}{2\pi a} \Big\{ & \text{mod} \left( \frac{1}{a} \Delta_x \theta_{\mathbf{r}}^h + gA_{\mathbf{r},x} \right) + \text{mod} \left( \frac{1}{a} \Delta_y \theta_{\mathbf{r}+\hat{x}}^h + gA_{\mathbf{r}+\hat{x},y} \right) \\ & - \text{mod} \left( \frac{1}{a} \Delta_x \theta_{\mathbf{r}+\hat{y}}^h + gA_{\mathbf{r}+\hat{y},x} \right) - \text{mod} \left( \frac{1}{a} \Delta_y \theta_{\mathbf{r}}^h + gA_{\mathbf{r},y} \right) \Big\}, \end{aligned} \quad (30)$$

where we have used the notation  $\text{mod}(x) = x \bmod 2\pi$ . This quantity has also been called the gauge invariant vortex density [4]. Looking at Eq. (30) we realize that it has the same form as  $A_{\square,\mathbf{r}}^f$  in Eq. (9) and can likewise be written as a plaquette sum. Defining the plaquette sum of a discrete vector field  $v_{\mathbf{r},\mu}$ , which both has a position  $\mathbf{r}$  and components  $\mu \in \{x, y\}$ , as

$$\sum_{\square_{\mathbf{r}}} v_{\mathbf{r},\mu} \equiv v_{\mathbf{r},x} + v_{\mathbf{r}+\hat{x},y} - v_{\mathbf{r}+\hat{y},x} - v_{\mathbf{r},y}, \quad (31)$$

then the local vorticity  $n_z^{(h)}$  can be written

$$n_z^{(h)}(\mathbf{r}) = \frac{1}{2\pi a} \sum_{\square_{\mathbf{r}}} \text{mod} \left( \frac{1}{a} \Delta_\mu \theta_{\mathbf{r}}^h + gA_{\mathbf{r},\mu} \right), \quad (32)$$

which is the form used in [8].

## References

- [1] Julien Garaud, Egor Babaev, Troels Arnfred Bojesen, and Asle Sudbø. Lattices of double-quanta vortices and chirality inversion in  $p_x + ip_y$  superconductors. *Phys. Rev. B*, 94(10):104509, Sep 2016.
- [2] Troels Arnfred Bojesen. *Large-scale Monte Carlo simulations of non-Abelian gauge theories and multicomponent superconductors*. PhD thesis, NTNU, 2014. 2014:252.
- [3] Peder Notto Galteland. *Monte-Carlo studies of multi-component Ginzburg-Landau theories with competing interactions*. PhD thesis, NTNU, 2016. 2016:214.
- [4] Akihiro Shimizu, Hidetoshi Ozawa, Ikuo Ichinose, and Tetsuo Matsui. Lattice ginzburg-landau model of a ferromagnetic  $p$ -wave pairing phase in superconducting materials and an inhomogeneous coexisting state. *Phys. Rev. B*, 85:144524, Apr 2012.
- [5] E. Smørgrav, J. Smiseth, E. Babaev, and A. Sudbø. Vortex sublattice melting in a two-component superconductor. *Phys. Rev. Lett.*, 94:096401, Mar 2005.
- [6] Eivind Smørgrav. *Critical propperties of effeffect gauge theories for novel quantum fluids*. PhD thesis, NTNU, 2005. :179.
- [7] Alexander Altland and Ben Simons. *Condensed Matter Field Theory*. Cambridge university press, 2010.
- [8] S. Kragset, E. Babaev, and A. Sudbø. Effects of boundaries and density inhomogeneity on states of vortex matter in bose-einstein condensates at finite temperature. *Phys. Rev. A*, 77:043605, Apr 2008.