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

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

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 $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$ is given in units of $\sqrt{2}B_C = \Phi_0/(2\pi\lambda\xi)$. The dimensionless gauge coupling used in the covariant derivatives $\mathbf{D} = \boldsymbol{\nabla} + ig\mathbf{A}$ 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 and third line shows what we call mixed gradient terms (MGT).

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

$$\eta^h \mapsto e^{i\lambda}\eta^h \tag{2a}$$

$$\mathbf{A} \mapsto \mathbf{A} - \frac{1}{g}\boldsymbol{\nabla}\lambda. \tag{2b}$$

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

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

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 completness.

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

$$\int \mathrm{d}^D x \mapsto a^D \sum_{\mathbf{r}}, \tag{4}$$

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 $\eta^\pm_{\mathbf{r}}, \eta^{\pm\,*}_{\mathbf{r}}$, 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

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

Note the abuse of vector notation in $\eta^h_{\mathbf{r}+\hat{\mu}}$ 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 Δ_μ becomes

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

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

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

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 2π periodicity and generally allows topologically nontrivial excitations such as magnetic monopoles [4] for large fluctuations of the vector potential.

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

$$F^{\mathrm{disc}} = F_K + F_{\mathrm{MGT}} + F_V + F_A. \tag{8}$$

The potential term is given by

$$F_V = a^2 \sum_{\mathbf{r}} \Big\{ \sum_h \big[-|\eta^h_{\mathbf{r}}|^2 + \frac{1}{2}|\eta^h_{\mathbf{r}}|^4 \big] + 2|\eta^+_{\mathbf{r}} \eta^-_{\mathbf{r}}|^2 + \nu\, \mathrm{Re}\left[(\eta^+_{\mathbf{r}})^{*\,2} (\eta^-_{\mathbf{r}})^2 \right] \Big\}, \tag{9}$$

while the Maxwell term F_A is given by the expression to the right in Eq. (7). The variables on the numerical lattice is assumed to be periodic - when e.g. $\eta^h_{\mathbf{r}+\hat{\mu}}$ 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

$$F_K = \sum_{\mathbf{r},\mu,h} \Big\{ 2|\eta^h_{\mathbf{r}}|^2 - \big[(\eta^h_{\mathbf{r}+\hat{\mu}})^* \eta^h_{\mathbf{r}} e^{-igaA_{\mathbf{r},\mu}} + \mathrm{c.c.} \big] \Big\}. \tag{10}$$

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

$$\begin{aligned}F_{\mathrm{MGT}} = \sum_{\mathbf{r}} \Big\{ &(\nu+1)\,\mathrm{Re}\left[\eta_{\mathbf{r}}^{-\,*}\big(\eta_{\mathbf{r}+\hat{y}}^{+} e^{igaA_{\mathbf{r},y}} - \eta_{\mathbf{r}+\hat{x}}^{+} e^{igaA_{\mathbf{r},x}}\big) + \eta_{\mathbf{r}}^{+}\big(\eta_{\mathbf{r}+\hat{y}}^{-\,*} e^{-igaA_{\mathbf{r},y}} - \eta_{\mathbf{r}+\hat{x}}^{-\,*} e^{-igaA_{\mathbf{r},x}}\big)\right] \\ &+(\nu-1)\,\mathrm{Im}\Big[\big(\eta_{\mathbf{r}+\hat{y}}^{+\,*}\eta_{\mathbf{r}+\hat{x}}^{-} - \eta_{\mathbf{r}+\hat{y}}^{-\,*}\eta_{\mathbf{r}+\hat{x}}^{+}\big)e^{iga(A_{\mathbf{r},x}-A_{\mathbf{r},y})} + 2\eta_{\mathbf{r}}^{+\,*}\eta_{\mathbf{r}}^{-} \\ &\qquad + \big(\eta_{\mathbf{r}}^{-\,*}\eta_{\mathbf{r}+\hat{x}}^{+} - \eta_{\mathbf{r}}^{+\,*}\eta_{\mathbf{r}+\hat{x}}^{-}\big)e^{igaA_{\mathbf{r},x}} + \big(\eta_{\mathbf{r}+\hat{y}}^{-\,*}\eta_{\mathbf{r}}^{+} - \eta_{\mathbf{r}+\hat{y}}^{+\,*}\eta_{\mathbf{r}}^{-}\big)e^{-igaA_{\mathbf{r},y}}\Big]\Big\}.\end{aligned} \tag{11}$$

The regularized free energy is invariant under the gauge-transformation

$$\eta_{\mathbf{r}}^{h} \mapsto e^{i\lambda_{\mathbf{r}}}\eta_{\mathbf{r}}^{h} \tag{12a}$$

$$A_{\mathbf{r},\mu} \mapsto A_{\mathbf{r},\mu} - \frac{\Delta_\mu \lambda_{\mathbf{r}}}{ga}. \tag{12b}$$

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. (8) yields the normal kinetic free energy

$$F_K^{\mathrm{lon}} = 2\sum_{\mathbf{r},\mu,h}\rho_h^2\Big\{1-\cos\big(\Delta_\mu\theta_{\mathbf{r}}^{h} + gaA_{\mathbf{r},\mu}\big)\Big\}, \tag{13}$$

the free energy given by the potential terms

$$F_V^{\mathrm{lon}} = a^2\mathcal{N}\Big\{\sum_h\big[-\rho_h^2 + \frac{1}{2}\rho_h^4\big] + (2-\nu)\rho_+^2\rho_-^2\Big\} + 2\rho_+^2\rho_-^2 a^2\nu\sum_{\mathbf{r}}\cos^2\big(\theta_{\mathbf{r}}^{+} - \theta_{\mathbf{r}}^{-}\big), \tag{14}$$

as well as the MGT free energy

$$\begin{aligned}F_{\mathrm{MGT}}^{\mathrm{lon}} = \rho_+\rho_-\sum_{\mathbf{r}}\Big\{&(\nu+1)\Big[\cos\big(\theta_{\mathbf{r}+\hat{y}}^{+} - \theta_{\mathbf{r}}^{-} + gaA_{\mathbf{r},y}\big) - \cos\big(\theta_{\mathbf{r}+\hat{x}}^{+} - \theta^{-}\mathbf{r} + gaA_{\mathbf{r},x}\big) \\ &+\cos\big(\theta_{\mathbf{r}+\hat{y}}^{-} - \theta_{\mathbf{r}}^{+} + gaA_{\mathbf{r},y}\big) - \cos\big(\theta_{\mathbf{r}+\hat{x}}^{-} - \theta_{\mathbf{r}}^{+} + gaA_{\mathbf{r},x}\big)\Big] \\ +(\nu-1)&\Big[\sin\big(\theta_{\mathbf{r}+\hat{x}}^{-} - \theta_{\mathbf{r}+\hat{y}}^{+} + ga(A_{\mathbf{r},x} - A_{\mathbf{r},y})\big) + \sin\big(\theta_{\mathbf{r}+\hat{y}}^{-} - \theta_{\mathbf{r}+\hat{x}}^{+} + ga(A_{\mathbf{r},y} - A_{\mathbf{r},x})\big) \\ &+2\sin\big(\theta_{\mathbf{r}}^{-} - \theta_{\mathbf{r}}^{+}\big) + \sin\big(\theta_{\mathbf{r}+\hat{x}}^{+} - \theta_{\mathbf{r}}^{-} + gaA_{\mathbf{r},x}\big) - \sin\big(\theta_{\mathbf{r}+\hat{x}}^{-} - \theta_{\mathbf{r}}^{+} + gaA_{\mathbf{r},x}\big) \\ &-\sin\big(\theta_{\mathbf{r}+\hat{y}}^{-} - \theta_{\mathbf{r}}^{+} + gaA_{\mathbf{r},y}\big) + \sin\big(\theta_{\mathbf{r}+\hat{y}}^{+} - \theta_{\mathbf{r}}^{-} + gaA_{\mathbf{r},y}\big)\Big]\Big\}.\end{aligned} \tag{15}$$

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.

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.