Supplementary material to "Unconventional states due to non-pairwise intervorex interactions in multicomponent superconductors"

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FINITE DIFFERENCE ENERGY MINIMIZATION

To calculate intervortex interaction energies we use finite difference energy minimization.

The GL free energy functional is

$$F = \frac{1}{2}\sum_{i=1,2}\left[|(\nabla + ie\mathbf{A})\psi_i|^2 + (2\alpha_i + \beta_i|\psi_i|^2)|\psi_i|^2\right] + \frac{1}{2}(\nabla\times\mathbf{A})^2 - \eta|\psi_1||\psi_2|\cos(\theta_2-\theta_1). \quad (1)$$

Ground states of vortex systems and inter-vortex interaction energies are found by minimizing this functional subject to relevant constraints, such as vortex positions.

To do this numerically, we discretize the system on a regular grid. To have the numerical results unbiased we use a non-adaptive grid where the grid spacing h is the same everywhere in the domain. The Hamiltonian is then discretized using the finite difference approach:

Gradients are defined as

$$(\nabla f)_{i,i+1} = \frac{f(i+1)-f(i)}{h} \quad (2)$$

and magnetic flux is computed by line integration

$$B_{i,i+1,j,j+1} = \frac{1}{h^2}\oint_\omega \bar{A}\cdot d\bar{r} \quad (3)$$

where ω is the square with the corners $i, i+1, j, j+1$. The energy density in the grid point (i,j) then depends on function values in i,j and its neighbors.

The optimization scheme which is used in the first part of the paper is a modified version of the Newton-Raphson method. There are 6 fields in the problem; real and imaginary parts of the complex fields and the two components of bfA. We denote these P. Optimization is conducted as follows:

1) Calculate dP

$$dP_i = -\frac{\partial E}{\partial P_i}\Big/\frac{\partial^2 E}{\partial P_i^2} \quad (4)$$

2) Test if dP lowers the energy, i.e. if $E(P+dP) < E(P)$. If this is the case, then we update $P \to P + dP$. Then, we move on to another grid point and attempt to update it. We generally find that the ratio of successful attempts to update the grid is close to 1. Thus, this differs from the usual Newton-Raphson scheme in two ways. First, we always check that the update indeed lowers the energy. Second, we do not compute the full matrix $\partial^2 E/\partial P_i \partial P_j$ but use only the diagonal elements.

To minimize boundary effects we use free boundary conditions. Vortices are inserted using various initial configurations.

In order to calculate the inter-vortex interaction energy, we have to fix the position of vortices. Fixing a vortex position requires a special care to avoid the situation where pinning to numerical grid substantially affects the vortex solution. We fix the vortex position by the following method. In the vortex center the condensate density is zero. We then fix the density only of the central point of the dominant component $|\psi_i|$ of the vortex to be zero in a given position of numerical grid. This effectively prevents the vortex from moving but does not prevent core splitting of $|\psi_1|$ and $|\psi_2|$ due to magnetic pressure. This "poin pinning" method also has advantage of being a "minimially invasive" since only the position of the core singularity is fixed. Thus it allows calculate medium- and long-range forces with greatest accuracy. However, at the same time, obviously, this method does not work for too short intervortex separation. For too short vortex separation it leads to the following easily identifiable artifact: a vortex core of one of the vortices elongates to be zero at both pinning centers allowing the second vortex to unpin and escape, while satisfying the energy minimization constraint. This behavior can be easily remedied by different pinning schemes but because short-distance vortex separation is irrelevant for the questions studied in this paper and also for consistency we use one pinning procedure.

The intervortex interaction obtained using this pinning scheme is consistent with the structure formation in unconstrained minimization obtained by two different methods in the second part of the paper.

Convergence is determined as follows:

1) We choose a particular grid spacing h_1 and number of grid points $N_1 = N_{1x}\cdot N_{1y}$ giving a system size $L_x = h\cdot(N_{1x}-1)$, $L_y = h\cdot(N_{1y}-1)$. Then we minimize the energy until it does not change in a few thousand iterations. This gives us $E(h_1)$.

2) We decrease grid spacing h by a factor of 2 or 3 while retaining the system size L_x, L_y using spline interpolation. Then, we once again iterate until the energy does not change in a few thousand iterations, giving us $E(h_2)$ and so forth. We then determine convergence from

$$\frac{E(h_n)-E(h_{n+1})}{E(h_n)} = C. \quad (5)$$

We use grid sizes up to $N \approx 10^7$ which gives very high accuracy, typically $C < 10^{-4}$.

FINITE ELEMENT ENERGY MINIMIZATION

In the second part of the paper we use the uncontrained energy minimization. Bound state vortex configurations are minima of Ginzburg-Landau energy (1). This means that functional minimization of (1), from an appropriate initial state describing several flux quanta, should lead to bound state (if it exists). We consider the two-dimensional problem $\mathcal{F} = \int_\Omega F$ defined on the bounded domain $\Omega \subset \mathbb{R}^2$, supplemented by free boundary conditions.

The variational problem is defined for numerical purpose using a finite element formulation provided by the Freefem++ [1] framework. Discretization within finite element formulation is done via a (homogeneous) triangulation on Ω, based on Delaunay-Voronoi algorithm. Functions are decomposed on a continuous piecewise quadratic basis on each triangle.

Contrary to the numerical method used in the first part, the accuracy does not depend only on the 'number of grid points'. The accuracy of such method is controlled through the number of triangles, (we typically used 10^5), the order of expansion of the basis on each triangle (P2 elements are 2nd order polynomial basis on each triangle), and also the order of the quadrature formula for the integral on the triangles.

Once the problem is mathematically well posed, a numerical optimization algorithm is used to solve the variational nonlinear problem (i.e. to find the minima of $\mathcal{F}$). We used here Nonlinear Conjugate Gradient method Algorithm is iterated until relative variation of the norm of the gradient of the functional $\mathcal{F}$ with respect to all degrees of freedom is less than 10^{-6}. To be sure that our results are not numerical artifacts of this particular minimization scheme, we also performed standard Steepest Descent calculations and checked it leads to similar results.

Minimization starts with an initial guess: a field configuration carrying the N_v flux quanta described by

$$\begin{aligned}
\Phi_a &= u_a \prod_{i=1}^{N_v} \sqrt{\frac{1}{2}\left(1 + \tanh\left(\frac{4}{\xi}(\mathcal{R}_i(x,y) - \xi)\right)\right)} \mathrm{e}^{i\Theta_i} \,, \\
\vec{A} &= \frac{1}{e\mathcal{R}} \left(\sin\Theta, -\cos\Theta\right) \,, \qquad (6)
\end{aligned}$$

where $a = 1, 2$, u_a is the vacuum expectation value of each scalar field, the parameter ξ gives the core size while Θ and $\mathcal{R}$ are

$$\begin{aligned}
\Theta(x,y) &= \sum_{i=1}^{N_v} \Theta_i(x,y) \,, \\
\Theta_i(x,y) &= \tan^{-1}\left(\frac{y - y_i}{x - x_i}\right) \,, \\
\mathcal{R}(x,y) &= \sum_{i=1}^{N_v} \mathcal{R}_i(x,y) \,, \\
\mathcal{R}_i(x,y) &= \sqrt{(x - x_i)^2 + (y - y_i)^2} \,. \qquad (7)
\end{aligned}$$

(x_i, y_i) are the initial position of a given vortex. Then, all degrees of freedom are relaxed simultaneously without *any* constraint to obtain high accurate solutions of the Ginzburg-Landau equations.

The initial guess (6) allows starting from various very different initial configurations, depending on the values of the (x_i, y_i). Since we know from two-body calculations, the preferred distance between two vortices, we choose to start either in the *repulsive* or in the *attractive* tail of the two-body interaction potential. Animations showing the evolution of the system from these various initial configurations is available in online supplementary material [2].

The method described in the first part of the paper was also used for unconstrained simulations to doublecheck some of the results.

[1] F. Hecht, O. Pironneau, A. Le Hyaric, and K. Ohtsuka, *Freefem++ (manual)* (2007) `www.freefem.org`.

[2] http://people.umass.edu/garaud/NonPairwise.html