Mesoscopics of half-quantum vortex pair deconfinement in a trapped spin-one condensate

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Motivated by a recent experiment in an antiferromagnetic spin-1 Bose-Einstein condensate of $^{23}\text{Na}$ atoms, we study the energetical stability of a singly quantum vortex injected into the center of a quasi-two-dimensional gas with zero total spin against dissociation into a pair of half-quantum vortices. We find that the critical dissociation point of this confinement-deconfinement type phase transition can be expressed in terms of the ratio of density-density ($c_0$) and spin-spin ($c_2$) coupling constants. The transition of bound to unbound vortices, in particular, sensitively depends on (1) the ratio of system size ($R$) to density healing length ($\xi_d$), and (2) the trap potential. Specifically, the critical ratio ($c_2/c_0)_c$ increases when $R/\xi_d$ decreases, and is relatively larger in a harmonic trap than in a box trap. Dissociation is energetically generally favored for $c_2/c_0 < (c_2/c_0)_c$, which as a corollary implies that vortex dissociation is observed as well for negative $c_2 < 0$, e.g., in a rubidium spin-1 BEC, whereas in a sodium spin-1 BEC ($c_2 > 0$) it is energetically blocked above the critical ratio ($c_2/c_0)_c$. Tuning the coupling ratio $c_2/c_0$ by using microwave control techniques, the dependence of the deconfinement phase transition on coupling parameters, density, and system size we predict, can be verified in experiments with ultracold spinor gases.

I. INTRODUCTION

Topological defects occur in Nature after a symmetry-breaking second-order phase transition $G \rightarrow H$, where $G$ is the original, larger symmetry group, and $H$ the remaining symmetry, whenever the homotopy group $\Pi_n(G/H)$ of the coset space $G/H$ is nontrivial [1]. Of particular interest in the context of condensed matter is the first homotopy group $\Pi_1$, the so-called fundamental group, which leads to vortices, around whose center the neutral or charged liquid is entrained to circulate according to the rule of flux quantization [2].

A particularly intriguing species of vortex defects in the order parameter texture are half-quantum vortices (HQVs), examples of which are furnished in $^3\text{He}$ [3–5] and spin-triplet superconductors [6, 7], polariton condensates [8, 9], as well as Bose-Einstein condensates (BECs) [10, 11]. The first observations of vortices in BECs [12–15] ignited intense research on these hallmarks of superfluid behavior and the condensate phase. The rich topology afforded by condensates with a multicomponent order parameter [14–18] then led, in particular, to various studies regarding the implementation and dynamical properties of HQVs in BECs, see, e.g., [19–24].

HQVs also occur in the realm of a quantum simulation of high-energy physics. In the latter, they feature under the name Alice strings [24–26]. Furthermore, within the context of particle-topological defect duality, the quark confinement–deconfinement transition has been described by the dissociation of a singly quantized vortex (SQV) into HQVs in spinor BECs [27] and in Rabi-coupled two-component condensates [28].

A confinement-deconfinement phase transition from a SQV into a pair of HQVs was recently observed in experiment [29], where the SQV was initially injected into a quasi-two-dimensional (quasi-2D) sodium BEC in the polar phase, then transferred to the antiferromagnetic (AF) phase, in which vortex dissociation was observed. The collisional dynamics of the HQVs was studied in [30]; also cf. the earlier experiments on quasi-2D skyrmions in [31]. The present theoretical study is motivated by the experimental observation on HQV deconfinement in an ultracold spin-1 Bose gas, and aims at gaining a deeper understanding of the physical mechanism behind the dissociation process [32], as well as to stimulate further experiments exploring the physics of HQV deconfinement.

HQV interactions have previously been studied in two-component condensates in the infinite system limit [33] [34]. Specifically, Ref. [33] found, under the condition $c_2 > 0$, at a critical point for which density-density ($c_0$) and spin-spin ($c_2$) coupling constants are equal, the vortex-antivortex force changes from repulsive ($c_2 < c_0$) to attractive ($c_2 > c_0$). Here, we consider a mesoscopically sized nonrotating spin-1 BEC in the AF phase, where the definition of mesoscopicity is afforded by the value of the ratio of system size $R$ to density-healing length $\xi_d$ ($\sim$ core size of SQV) being finite, to reveal the intricate interplay of density-density and spin-spin interactions in the vortex dissociation process. We also demonstrate how the finite-size geometry helps us to reveal finer details of the physical origin of confinement versus deconfinement. In particular, we go beyond the study presented in [33] by considering (1) a finite size, mesoscopic gas, (2) both box and harmonic trap potentials, and (3) both positive and negative spin-spin coupling, $c_2 > 0$ and $c_2 < 0$, respectively. Our results are thus applicable to both sodium [35] respectively rubidium [36] spin-1 condensates. Due to the definition of the density-density interaction coupling, $c_0 > 0$, for any spin-1 BEC in the thermodynamic limit to be stable [13]. Denoting $n$ the mean 3D number density of the spin-1 BEC, in a homogeneous gas, the ground state is...
the AF phase if $|p| < c_{2n}$, $q < 0$, and $c_{2} > 0$ [15]. We then take as a working hypothesis below that the phase diagram of the finite-size spin-1 BEC containing vortices is qualitatively similar (within our parameter regimes) to that of the infinite homogeneous spin-1 BEC.

To create vortices in the spin-1 BEC, one needs to disturb it by (sufficiently rapidly) rotating it [12] or by dragging a repulsive Gaussian laser beam through the gas [33]. In a repulsive Gaussian laser beam the gas, $E_{\text{ret},ij} < E_{V,j}$ where $E_{\text{ret},ij}$ is the total energy in a phase $j$ without vortex and $E_{V,j}$ is the energy in that same phase with vortices present. However, due to topological conservation laws, once the vortex is created above the ground state, it will decay slowly to the ground state containing no vortex. Our aim is to derive the energetical stability against vortex dissociation from a SQV to a pair of HQVs in a quasi-2D spin-1 BEC; we assume as an axially symmetric initial condition that a SQV has been created at the center of the system. A BEC with two oppositely charged HQVs does not represent the ground state as well. Nevertheless, this configuration is potentially more stable than a BEC with a SQV, thus the dissociation from a SQV to two oppositely charged HQVs can be observable [29].

II. GENERAL SETUP AND METHOD

A. Hamiltonian

Two vortices with equal supercurrent winding numbers $q_{n}$ (see Def. [9] below) rotate around each other with the center of mass being fixed, which has been verified for half-quantum vortices spin-1 BECs in [34]. To facilitate our calculations, we therefore use a co-rotating frame of two HQVs symmetrically placed at $(x, y) = (\pm D/2, 0)$. Also, when we calculate the energy of the system with a SQV, for the same reason of retaining a sufficient degree of spatial symmetry, we assume that the SQV is at the center of the system. Then, the Hamilton operator generally transforms according to $\hat{H} \rightarrow \hat{H} - \Omega \cdot \hat{L}$, with $\hat{\Omega} \cdot \hat{L} = -i\hbar \Omega (\partial/\partial \varphi)$ where $\hat{\Omega} = \Omega_{\hat{z}}$ is the angular velocity of the two co-rotating HQVs with respect to their center of mass (origin of coordinates), $\hat{L}$ is an angular momentum operator, and $\varphi$ the azimuthal angle. Therefore, due to cylindrical symmetry, the Hamiltonian with a SQV at the center remains invariant when going to the rotating frame. Using this fact, we may use the Hamilton operator for a nonrotating spin-1 BEC to calculate the energetical stability of the vortex dissociation process. The Hamilton operator is given by [15]

$$
\hat{H} = \int d^{3}r \left[ -\frac{\hbar^{2}}{2M} \nabla^{2} + V_{\text{trap}}(r) - \mathbf{p} \cdot \mathbf{f} + q \mathbf{f}_{z} \right] \hat{\psi} \\
+ \frac{1}{2} \int d^{3}r \left[ c_{0} (\hat{\psi}^{\dagger} \hat{\psi})^{2} + c_{2} (\hat{\psi}^{\dagger} \mathbf{f} \hat{\psi}) \cdot (\hat{\psi}^{\dagger} \mathbf{f} \hat{\psi}) \right],
$$

(1)

where $\hat{\psi}$ is the three-component spinor field operator and $V_{\text{trap}}$ represents the scalar trapping potential, cf. Eq. [3] below. The coupling constants for density-density and spin-spin interactions are, respectively, $c_{0} = (g_{0} + 2g_{2})/3$ and $c_{2} = (g_{2} - g_{0})/3$, where $g_{i} = 4\pi \hbar^{2} a_{\text{a}}/M$. Here, $M$ is the mass of gas constituents, and $a_{\text{a}}$ is the s-wave scattering length of the spin-$\mathcal{F}$ channel in units of the Bohr radius $a_{B}$. Furthermore, $\hat{\mathbf{f}}$ is the spin-1 operator so that $(\hat{f}_{z})_{m,m'} = m \delta_{m,m'} \left( m, m' = -1, 0, 1 \right)$ where $\delta_{m,m'}$ is the Kronecker delta. The operator of the total spin in $z$ direction is given by the integral of the spin density as [37]

$$
\hat{S}_{z} = \hbar \int d^{3}r \hat{\psi}^{\dagger} \mathbf{f}_{z} \hat{\psi},
$$

(2)

and commutes with the Hamilton operator in Eq. [1], so that the integral of the magnetization, the total magnetic moment (obtained by multiplying $S_{z}$ with the magnetic moment of the spin-1 boson) is conserved. Also, $p$ denotes the linear Zeeman coefficient, and $q$ its quadratic counterpart.

We operate with negative quadratic Zeeman shift, $q < 0$. According to [1], the quadratic Zeeman energy is $q \int d^{3}r (\hat{\psi}^{\dagger}_{1} \hat{\psi}_{1} + \hat{\psi}^{\dagger}_{-1} \hat{\psi}_{-1})$ where $\hat{\psi}_{m}$ is the component of $\hat{\psi}$ with magnetic quantum number $m_{z} = m$. Therefore, for sufficiently large negative $q < 0$, and independent of the sign and magnitude of $c_{2}$, the total energy is lowered when $\hat{\psi}_{0} \rightarrow 0$ because of the conservation of the norm of $\hat{\psi}$. Assuming vanishing total spin, $\hat{S}_{z} = 0$, the ground state is then the AF phase, which leads to the wavefunction ansatz in Eq. [5] below.

Note that for negative spin-spin coupling $c_{2} < 0$, ferromagnetic domains might potentially occur. However, within our subspace of vanishing total spin, we have verified that for the relatively small $|c_{2}/c_{0}| \sim \mathcal{O}(1)$ we consider, the formation of ferromagnetic domains is energetically disfavored.

Finally, because our focus is on spinor gases in the AF phase and [1] becomes independent of $p$ when $\hat{S}_{z} = 0$, we fix $p = 0$ to facilitate our calculations, as $p$ is rendered dynamically irrelevant within a subspace of conserved vanishing total spin.

B. Dimensional reduction

We assume that a mean-field description of the quantum gas is applicable. Hence we replace the spinor field operator in [1] by its mean field, $\hat{\psi}$.

We consider the two types of trap potential experimentally commonly realized: harmonic and box traps. To capture both within a single formula, the scalar potential in [1] is assumed to be of the form

$$
V_{\text{trap}}(r, z) = \left\{ \begin{array}{ll}
\frac{1}{2} M \omega^{2} r^{2} + \frac{1}{2} M \omega_{z}^{2} z^{2} \quad & \text{if } r < R \\
\infty \quad & \text{if } r \geq R
\end{array} \right.
$$

(3)

with $\omega > 0$ and $\nu \geq 0$. Here, $\mathbf{r}$ is the position vector in the $x$-$y$ plane, and $r := |\mathbf{r}|$. For this trap potential, we
define scaled variables according to
\[
\tau := i\omega t, \quad \hat{r} := \frac{r}{l}, \quad l = \sqrt{\frac{\hbar}{M\omega}}.
\] (4)

Here, \(\omega\) is a scaling frequency in the \(x\)-\(y\) plane. For the box trap, we may set \(\omega\) to have an arbitrary value, and \(\nu = 0\). For a harmonic trap with \(\omega_\perp\) the angular frequency of the harmonic trap in the \(x\)-\(y\) plane, let \(R_{\text{TF}}\) be the Thomas-Fermi (TF) radius of the system in \(x\)-\(y\) plane. We may then set \(\nu = \omega_\perp/\omega\) and the system size is redefined as \(R = R_{\text{TF}} + \delta R\) where \(\delta R\) is a nonnegative value introduced to aid the convergence of the numerical calculation. We therefore define \(R := R/l\).

For a quasi-2D spin-1 BEC, we employ the following ansatz for an AF mean-field wavefunction \(\psi(r, t)\),
\[
\psi = \sqrt{\frac{N}{2l_z^2\sqrt{\pi}}} e^{-i((\omega_1/2)+(q/\hbar)t_1)e^{-z^2/(2l_z)^2}} \tilde{F}(\hat{r}, \varphi, \tau),
\]
\[
\tilde{F}(\hat{r}, \varphi, \tau) = [-\hat{f}_1(\hat{r}, \varphi, \tau) \ 0 \ \hat{f}_{-1}(\hat{r}, \varphi, \tau)]^T,
\] (5)

where \(l_z = \sqrt{\hbar/(M\omega_z)}\) is the harmonic oscillator length along the \(z\) axis and \(N\) is the number of BEC atoms or molecules. The normalization condition is \(\int d^3r |\psi|^2 = N\), and \(\int d^3r \psi^* \psi = 0\) because \(S_z = 0\). Here, \(\hat{f}_m(\hat{r}, \varphi, \tau)\) are complex functions.

Then, by assuming the transverse \(z\) direction to be frozen to the harmonic oscillator ground state \([\Psi_0]^{40}\) and correspondingly integrating it out, for \(r < R\) the following effective quasi-2D equations are obtained:
\[
-\frac{\partial \hat{f}_{\pm 1}}{\partial \tau} = \left[-\frac{1}{2} \tilde{\nabla}_{2D}^2 + \frac{1}{2} v_\perp^2 r^2 \right] \hat{f}_{\pm 1} + NC \left[ \left( c_0' + c_2' \right) \hat{f}_1^2 + \left( c_0' - c_2' \right) \hat{f}_{-1}^2 \right] \hat{f}_{\pm 1},
\]
\[
\int_0^{2\pi} d\varphi \int_0^R d\hat{r} \hat{r} \hat{f}_1^2 = \int_0^{2\pi} d\varphi \int_0^R d\hat{r} \hat{r} \hat{f}_{-1}^2 = \frac{1}{2}
\] (6)

In Eq. (6), \(\tilde{\nabla}_{2D} := (\partial/\partial \hat{r}) \hat{e}_r + (1/\hat{r}) (\partial/\partial \varphi) \hat{e}_\varphi\) where \(C := 2\sqrt{2\pi} (a_B/l_z)\), \(c_0' := (a_0 + 2a_2)/3\), and \(c_2' := (a_2 - a_0)/3\). For \(\hat{r} \geq R\), \(\hat{f}_m = 0\).

By virtue of Eq. (6), the density healing length \(\xi_d\) satisfies
\[
R/\xi_d = \sqrt{\frac{2}{\pi}} NC c_0' = \sqrt{\frac{2M c_0}{\hbar^2}} \frac{N}{\pi (l_z^2/2\pi)}
\] (7)

and for \(\nu \neq 0\), the TF radii \(R_{\text{TF}}\) have the form
\[
R_{\text{TF}} = \frac{l}{\sqrt{C}} \sqrt{\frac{4}{\pi}} NC c_0' = l_\perp \sqrt{\frac{4}{\pi}} NC c_0',
\] (8)

where \(l_\perp = \sqrt{\hbar/(M\omega_\perp)}\) is harmonic oscillator length in the \(x\)-\(y\) plane. Using Eq. (7) for a quasi-2D system, we may define the volume of the BEC as \((4\pi R^2/3) \left(3\sqrt{2\pi}l_z/4\right)\). Specific values of \(\omega_\perp\) and \(R\) for harmonically trapped gases will be introduced in section [III.B]

C. General Ansatz for up to Two Vortices

We now (1) present our ansatz to calculate the wavefunction of the spin-1 quasi-2D BEC in the AF phase, with up to two vortices with opposite spin windings and (2) establish an energy criterion for vortex dissociation, by defining the (scaled) energy difference Eq. (10) below. To this end, we first expound our general ansatz employed when quantum vortices are present in the system, which proved beneficial to reduce the computational time for both box (see section III.A) and harmonic traps (see section III.B)

1. Vortex ansatz in the AF phase

We denote \(q_{su}\) as the supercurrent winding number, and \(q_{su}\) as the spin winding number \([15, 29]\), where, with the line integral taken around the central singularity in the vortex core,
\[
\oint d\mathbf{l} \cdot \mathbf{v}_s = \frac{2\pi \hbar}{M} q_{su}, \quad \oint d\phi_s = 2\pi q_{su}.
\] (9)

Here, \(\phi_s\) is the azimuthal angle of spin orientation in the AF phase, \(M\) is the mass of bosons, and \(v_s := (\hbar/M) \text{Im} (\psi^\dagger \nabla \psi)\) is the superfluid velocity.

In order to consider a vortex pair containing a \((q_s, q_{su}) = (Q_n, Q_s)\) vortex, whose core is at \(\tilde{r}\), \(\phi\) and \((q_s, q_{su}) = (Q_s, -Q_n)\) vortex, whose core is located at \(\tilde{r}\), \(\phi\), we use the following ansatz:
\[
\tilde{f}_{\pm 1}(\tilde{r}, \phi, \tau) = \tilde{A}_{\pm 1}(\tilde{r}, \phi, \tau) \times \exp \left\{ i \left[ \Phi_{\pm 1}(\tilde{r}, \phi) + \Theta_{\pm 1}(\tilde{r}, \phi) + \tilde{B}_{\pm 1}(\tau) \right] \right\},
\] (10)

where \(\Phi_{\pm 1}(\tilde{r}, \phi) := (Q_n \mp Q_s) \phi_F(\tilde{r}, \phi), \Theta_{\pm 1}(\tilde{r}, \phi) := (Q_n \pm Q_s) \phi_G(\tilde{r}, \phi),\) and
\[
\cos \phi_F(\tilde{r}, \phi) := \frac{\tilde{r} \cos \phi - \tilde{r}_F \cos \phi_{\pm 1}}{\sqrt{\tilde{r}^2 + (\tilde{r}_F)^2 - 2\tilde{r} \tilde{r}_F \cos (\phi - \phi_{\pm 1})}},
\]
\[
\cos \phi_G(\tilde{r}, \phi) := \frac{\tilde{r} \cos \phi - \tilde{r}_G \cos \phi_{\pm 1}}{\sqrt{\tilde{r}^2 + (\tilde{r}_G)^2 - 2\tilde{r} \tilde{r}_G \cos (\phi - \phi_{\pm 1})}}.
\] (11)

Here, \(\tilde{A}_{\pm 1}\) and \(\tilde{B}_{\pm 1}\) are some real functions. Due to the single-valuedness of the wavefunction, \(Q_n \pm Q_s\) should be integer. Then, the superfluid velocity \(V_s\) becomes
\[
V_s = \frac{\hbar}{Ml} \sum_{m = \pm 1} \left\{ \tilde{\nabla}_{2D} \left( \Phi_m + \Theta_m \right) \right\} \tilde{A}_m^2.
\] (12)

For the present system with radius \(R\), let \(\Phi_{\pm 1}\) be the phase of the image vortex of the \((Q_n, Q_s)\) vortex at
\[(\tilde{r}, \tilde{\varphi}) = (\tilde{r}_F, \varphi_F).\]  
In order to make the radial component of superfluid velocity vanish at the boundary, one imposes

\[
\begin{align*}
\Phi'_{\pm 1}(\tilde{r}, \varphi) &= -(Q_n \mp Q_s) \phi'_{\pm 1}(\tilde{r}, \varphi), \\
\cos \phi'_{\pm 1}(\tilde{r}, \varphi) &= \frac{\tilde{r} \cos \varphi - \tilde{r}_F \cos \varphi_F}{\sqrt{\tilde{r}^2 + (\tilde{r}_F)^2 - 2\tilde{r}\tilde{r}_F \cos(\varphi - \varphi_F)}},
\end{align*}
\]

where \(\tilde{r}_F = \tilde{R}/\tilde{r}_F\) if \(\tilde{r}_F \neq 0\). Observe that when \(\tilde{r}_F = 0\), the \((Q_n, Q_s)\) vortex is at the center of the system. Hence there is no radial component of superfluid velocity at the boundary of the system with radius \(R\) and no image vortex is required to satisfy the boundary conditions. Likewise, we define \(\Theta_{\pm 1}\) as the phase of the image vortex of the \((Q_n, -Q_s)\) vortex at \((\tilde{r}, \varphi) = (\tilde{r}_G, \varphi_G)\).

When there is only one vortex with \((q_n, q_s) = (Q_n, Q_s)\) at the center, \(\phi_G = \phi_F = \Theta_{\pm 1} = \Theta'_{\pm 1} = 0\). When there is only one vortex with \((q_n, q_s) = (Q_n, Q_s)\) off the center, \(\phi_G = \phi_F = \Theta_{\pm 1} = \Theta'_{\pm 1} = 0\). Finally, if there is no vortex, \(\phi_F = \phi_G = \Theta_F = \Theta_G = \Theta'_{\pm 1} = \Theta'_{\pm 1} = 0\).

Employing the ansatz Eq. \((10)\), the first line of Eq. \((6)\) takes the form

\[
\begin{align*}
-\frac{\partial \tilde{A}_{\pm 1}}{\partial \tilde{r}} &= \left[ -\frac{1}{2} \nabla^2_{2D} + \frac{1}{2} \nabla_{2D} \left( \Phi_{\pm 1} + \Phi'_{\pm 1} + \Theta_{\pm 1} + \Theta'_{\pm 1} \right) \right] \tilde{A}_{\pm 1}, \\
\tilde{A}_{\pm 1} &= \left[ \nabla_{2D} \left( \Phi_{\pm 1} + \Phi'_{\pm 1} + \Theta_{\pm 1} + \Theta'_{\pm 1} \right) \right] \cdot \nabla_{2D} + \frac{1}{2} \left( \nabla^2_{2D} \left( \Phi_{\pm 1} + \Phi'_{\pm 1} + \Theta_{\pm 1} + \Theta'_{\pm 1} \right) \right) \tilde{A}_{\pm 1},
\end{align*}
\]

where \(H_{\pm 1} := \frac{1}{2} \nu^2 \tilde{r}^2 + NC \left( \left( c_0^2 + c_0^2 \right) \tilde{A}_{\pm 1} \right) \) and \(\int_0^{2\pi} d\varphi \int_0^\tilde{R} d\tilde{r} \tilde{r} \tilde{A}_{\pm 1}^2 = \frac{1}{2} \). (14)

and

\[
\begin{align*}
\frac{E}{N} &= \frac{\hbar \omega}{2} \int_0^{2\pi} d\varphi \int_0^\tilde{R} d\tilde{r} \tilde{r} \sum_{m=\pm 1} \left[ \left( \nabla_{2D} \tilde{A}_m \right)^2 + \left( \nabla_{2D} \left( \Phi_{\pm 1} + \Phi'_{\pm 1} + \Theta_{\pm 1} + \Theta'_{\pm 1} \right) \right)^2 + \nu^2 \tilde{r}^2 \right] \tilde{A}_m^2 \\
&+ \frac{\hbar \omega}{2} \int_0^{2\pi} d\varphi \int_0^\tilde{R} d\tilde{r} \nu NC \left[ c_0' \left( \tilde{A}_{\pm 1}^2 - \tilde{A}_{\pm 1}^2 \right)^2 + c_2' \left( \tilde{A}_{\pm 1}^2 - \tilde{A}_{\pm 1}^2 \right)^2 \right] + q + \frac{\hbar \omega_z}{4},
\end{align*}
\]

where \(E\) is the total energy of the system in the AF phase, according to Eqs. \((6)\) and \((10)\). Since the squared amplitude fulfills \((L_z \sqrt{\pi}) |\psi_{\pm 1}(x, y, z, t)|^2 = N e^{-(\nu l_z)^2} |\tilde{f}_{\pm 1}(\tilde{x}, \tilde{y}, \tilde{z})|^2 \) and \(\tilde{B}_{\pm 1}\) does not affect the density profile of the gas. Also, it does not affect the superfluid velocity, see \((12)\) and the Hamiltonian \((1)\). We therefore omit the \(\tilde{B}_{\pm 1}\) term in what follows.

2. Definition of scaled energy difference

Let \(E_{\text{ref}}\) be the total energy without vortex, \(E_S\) be that with a SQV at the center, and \(E_H\) be that with two oppositely charged HQVs, each at \((x, y) = (\pm D/2, 0)\). According to Eq. \((15)\), as \(Nq + N\nu \omega_z/4\) does not depend on \(\tilde{A}_{\pm 1}\), when we assess the energetical stability against vortex dissociation we examine the behavior of the (scaled) energy difference

\[
\Delta E_{H,S} := \left( \tilde{E}_H - \tilde{E}_S \right) / \tilde{E}_{\text{ref}}, \quad (16)
\]

where the shifted energies \(\tilde{E}_{\text{ref}} := E_{\text{ref}} - Nq - N\nu \omega_z/4, \tilde{E}_S := E_S - Nq - N\nu \omega_z/4, \) and \(\tilde{E}_H := E_H - Nq - N\nu \omega_z/4.\) Hence, the exact value of \(q\) is immaterial, as it does not appear in Eq. \((14)\) and in the (scaled) energy difference defined above.

D. Numerical Method

The numerical method to solve Eq. \((14)\) is based on Refs. \((41, 42)\), which employ a second-order splitting method (so-called Strang splitting) \((43)\), to separate linear and nonlinear terms in the GP (Gross-Pitaevskii) equation. In order to ensure that \(S_z\) is conserved, a projection constant was introduced. As \(\psi_0 = 0\), the projection constant for \(\psi_{\pm 1}\) becomes the normalization factor of \(\psi_{\pm 1}\). In \((40)\) \((41)\), a similar procedure was used to solve the scalar GP equation.

A graphics processing unit (GPU) has thousands of cores which can perform a parallel computation only if one uses specific computing language. Supercomputers are capable of performing parallel computation, but one needs to assign the workloads to nodes which are parts of the supercomputer. Therefore, to reduce the total computing time by using parallel processing, we wrote two codes: one with OpenCL to use a GPU of AMD, and another code using a message passing interface (MPI) to
take advantage of a supercomputer for solving Eq. (14).

We studied gases trapped in box and harmonic trap potentials, whose form is given in Eq. (3), fixing \( \omega_\perp / 2 \pi = 400 \) Hz (as employed in the sodium experiments [29]). The mass \( M \) used for \(^{23}\text{Na}\) atoms and \( c_0^\text{H} \) is fixed to be 51.1, which corresponds to the bare \( c_0^\text{H} \) value of \(^{23}\text{Na} \) [15]. We limited the pair size to \( D < 2R \) where \( R \) is the distance between the two oppositely charged HQVs, because, naturally, physical vortex cores are located within the gas cloud. According to Eq. (7), \( R/\xi \) (see Eq. (3)), is the distance between the two oppositely charged HQVs, because, naturally, physical vortex cores are located within the gas cloud. According to Eq. (7), \( R/\xi \) is determined from Eq. (7) and for a quasi-2D spin-1 gas of \(^{23}\text{Na} \) atoms. The relation between \( \omega_\perp \) and \( \omega_\parallel \) is given in Eq. (3), fixing \( \omega_\parallel / \pi = 0.0907 \sqrt{N} \). Note that \( R/\xi_d \) does not depend on \( \omega_\perp \). Therefore, once we set \( R/\xi_d \), it is not necessary to change \( N \) irrespective of whether the trap is a box or harmonic one. Table I displays the set of \( R/\xi_d \) and \( N \) values used in this paper, together with the in-plane trap frequency \( \omega_\perp \).

We posit that \( \tilde{A}_m (\tau = \tau_0) \) is the ground state solution of Eq. (14) if it satisfies the inequality

\[
\int d^2 \tilde{r} \sum_{m=1}^{d} \left[ \tilde{A}_m (\tau = \tau_1) - \tilde{A}_m (\tau = \tau_0) \right]^2 < \epsilon,
\]

where \( \tau_1 = \tau_0 + d\tau \) and \( \epsilon \) is some small positive number which determines the convergence of the solution of Eq. (14). \( d\tau > 0 \) represents the imaginary time step size. Then, since our ground state criterion in Eq. (14) includes spatial integration, as \( \tilde{R} \) decreases, \( \epsilon \) should be decreased as well so that our ground state criterion is consistent independent of \( \tilde{R} \). In other words, we consider \( \tilde{A}_m (\tau = \tau_1) \) to be the ground state solution if it satisfies the following inequality,

\[
\frac{1}{\pi \tilde{R}} \int_0^{2\pi} d\varphi \int_{\tilde{r}}^{\tilde{R}} d\tilde{r} \sum_{m=1}^{d} \left| \tilde{A}_m (\tau = \tau_1) - \tilde{A}_m (\tau = \tau_0) \right|^2 < \tilde{\epsilon}.
\]

Here, \( \tilde{\epsilon} \) is another small number, set to be of the order of the typical machine precision, \( \tilde{\epsilon} = \mathcal{O}(10^{-14}) \).

Defining \( \Delta \tilde{r} > 0 \) as the step size of \( \tilde{r} \), and \( \Delta \varphi > 0 \) as the step size of \( \varphi \), when \( \xi_d \) decreases, both \( \Delta \tilde{r} \) and \( \Delta \varphi \) are required to remain small, because the numerical solutions of Eq. (14) diverge if \( \Delta \tilde{r} \geq \min (\xi_d, \xi_\parallel) / l \) or \( \Delta \varphi \geq \min (\xi_d, \xi_\parallel) \), where \( \min (a, b) = a \) if \( a \leq b \) and \( b \) if \( a > b \). Here, \( \xi_\parallel \) satisfies \( R/\xi_\parallel = \sqrt{2NC^r_2}/\pi \) by generalizing Eq. (7) with \( \xi_d \).

Given our numerical resources, we can study system sizes up to \( R/\xi_d = 8 \). In addition, when limiting the numerical calculation time, there is a restriction on \( c_2/c_0 \): When \( c_0 > 0 \), Eq. (14) effectively decouples when \( c_2 = c_0 \), whereas the coupling of \( \tilde{A}_1 \) and \( \tilde{A}_{-1} \) increases as \( c_2 < c_0 \) or \( c_2 > c_0 \). Therefore, it is more time-consuming to solve Eq. (14) for \( c_2/c_0 \neq 1 \). Hence, limit ourselves to \(-0.5 \leq c_2/c_0 \leq 2 \) given the resources.

### III. DECONFINEMENT OF HALF-QUANTUM VORTICES

#### A. Box Traps

When we consider box traps, \( \nu = 0 \) in Eq. (14). Also, there is no constraint imposed on \( R \) like for harmonic traps: Once \( N \) is determined, \( R/\xi_d \) is automatically determined by Eq. (7). Similarly, \( R/\xi_\parallel \) is also determined by \( c_2 \). Note that our ansatz, Eqs. (5) and (14), is valid for \( 0 \leq \tilde{r} < \tilde{R} \) [see Eq. (3)], where \( \tilde{R} \) is the harmonic oscillator type length scale which depends on the “scaling frequency” \( \omega_\parallel \), as introduced below Eq. (3). Therefore, to assess the energetics of vortex dissociation for box trap potentials, we may select one specific value of \( R \). For example, suppose that one has solved Eq. (14) for the system (Sys1) with box trap potential and \( R = R_{\text{Sys1}} \) be the scaled system size. Let \( E - Nq - N\omega_\parallel \) for that system be \( \tilde{E}_{\text{Sys1}} \). Then, using Eq. (15), one finds for system Sys2 an energy expression equivalent to changing the spatial size of Sys1 by a factor \( a \), \( \tilde{E}_{\text{Sys2}} = \tilde{E}_{\text{Sys1}} / a^2 \). Using this feature, to reduce computing time, we therefore set \( \omega_\parallel / 2 \pi = 5 \) Hz to scale lengths in units of \( l = 9.37 \) \( \mu m \), and set \( \tilde{R} = 0.2 \).

To assess the dependence of the energetical stability against vortex dissociation on \( (R/\xi_d, c_2/c_0) \), we fix \( R/\xi_d = 4 \) and \( c_0 > 0 \), and obtained the data in Fig. 1 (a). One observes that \( \Delta E_{H,S} \) has a critical value \( (c_2/c_0)_{cr} \) where the dissociation becomes unfavorable for \( c_2/c_0 > (c_2/c_0)_{cr} \). It has previously been established that the critical value \( (c_2/c_0)_{cr} = 1 \) for an infinitely large sys-

![FIG. 1. Scaled energy difference \( \Delta E_{H,S} \) as a function of \( c_2/c_0 \) for (a) \( R/\xi_d = 4 \), (b) \( R/\xi_d = 8 \) with box trap. Black dots are for \( D/\xi_d = 1 \), blue dots are for \( D/\xi_d = 2 \), and red dots are for \( D/\xi_d = 4 \), indicating how the energetical stability against vortex dissociation depends on \( c_2/c_0 \). The force between two oppositely charged HQVs are repulsive for every \( c_2/c_0 \) region in this figure. The inset shows the critical crossing of \( c_2/c_0 \) for \( D/\xi_d = 1 \); horizontal and vertical axis are identical to the main plot.](image-url)
FIG. 2. $\Delta \bar{E}_{H,S}$ for various $c_2/c_0$ with box trap. The upper panel shows $\Delta \bar{E}_{H,S}$ along the $x/\xi_d$ axis, and the lower panel displays 2D contour plots of $\Delta \bar{E}_{H,S}$. The critical values $(c_2/c_0)_{cr}$ are 1.9 and 1.2 for $R/\xi_d = 4$ and 8 with box trap, respectively. As $c_2/c_0$ decreases, $\Delta \bar{E}_{H,S}$ decreases due to the spin interaction energy.

From Fig. 1 as $R/\xi_d$ decreases, the critical value of $c_2/c_0$ is expected to be shifted to larger $c_2/c_0$ value. To check whether this expectation is true, we set $R/\xi_d = 8$ and changed $c_2$ while fixing $c_0$. Figure 1(b) shows that $(c_2/c_0)_{cr}$ value is about 1.2, but it is larger than $(c_2/c_0)_{cr}$ for $R/\xi_d \rightarrow \infty$. Therefore, our assumption that $(c_2/c_0)_{cr}$ is shifted to smaller value as $R/\xi_d$ increases is true for $4 \leq R/\xi_d \leq 8$. These results are consistent with the harmonic trap data (see section below), we summarize the critical $(c_2/c_0)_{cr}$ values in table I.

To determine how $R/\xi_d$ affects $(c_2/c_0)_{cr}$, as $(c_2/c_0)_{cr}$ is determined by comparing $E_H$ and $E_S$, we correspondingly compared the (scaled) energy density for various $R/\xi_d$ and $c_2/c_0$. Here, Eq. (17) defines the (scaled) energy density $\Delta \bar{E}_{H,S}$:

$$\Delta \bar{E}_{H,S} = \int_0^{2\pi} d\phi \int_0^{R_d} dr_d r_d \Delta \bar{E}_{H,S}. \quad (17)$$

Here, $r_d := r/\xi_d$ and $R_d := R/\xi_d$. Note that $\Delta \bar{E}_{H,S}$ is dimensionless due to the definition of $\Delta \bar{E}_{H,S}$. Eq. (16). Fig. 2 shows $\Delta \bar{E}_{H,S}$ for $R/\xi_d = 4$ and 8 when $D/\xi_d = 1$.

Because $E_S$ and $E_{red}$ do not depend on $c_2$ with a SQV in the AF phase [27], solely HQVs affect the shape of $\Delta \bar{E}_{H,S}$ when $c_2/c_0$ changes. As one can see from Fig. 2, the energy density with HQVs is concentrated in their cores whereas it strongly decreases near the center when $c_2/c_0$ increases. This is due to the combined effects of spin interaction energy, kinetic energy, and the phases of two oppositely charged HQVs. Since we assumed that two HQVs with $(q, q_a) = (1/2, \pm 1/2)$ are symmetrically placed at $(x, y) = (\pm \xi_d/2, 0) \quad (D = \xi_d)$, for $c_2 \rightarrow \infty$ keeping $c_0$ fixed, from symmetry, normalization and total spin constraints, the following conclusions can be drawn: (1) The spin healing length $\xi_s \propto 1/\sqrt{c_2}$ and the core size of a HQV decreases upon increasing $c_2$. Then, from [20], in-between the cores of the two HQVs, the kinetic and spin interaction energy densities decrease to negligibly small values, and the density-density interaction contribution becomes constant. (2) While the spin interaction energy tends to minimize the difference of $A_{\pm 1}$ when $c_2 > 0$, due to phase constraints, $A_1^2 - A_{-1}^2$ cannot be zero near the cores of HQVs. Hence, the spin interaction energy density in the cores of HQVs increases. Therefore, the double peaks in $\Delta \bar{E}_{H,S}$ become increasingly narrow when $c_2/c_0$ increases, which leads to $\Delta \bar{E}_{H,S} > 0$ for $c_2/c_0 > (c_2/c_0)_{cr}$. For smaller $R/\xi_d$, the cores of HQVs become relatively larger. As a result, $c_2/c_0$ must increase to make the peaks in $\Delta \bar{E}_{H,S}$ more narrow. This constit-
tutes the reason for \((c_2/c_0)_{cr}\) being increased when \(R/\xi_d\) decreases.

**B. Harmonic Trapping**

We now consider a harmonic trap potential in the \(x\)-\(y\) plane. In a quasi-2D spinor gas with \(\omega_x = \omega_y = \omega_z > 0\), we have \(\omega_z \ll \omega_x\). Setting \(\omega = \omega_x\), we have \(\nu = 1\) in Eq. (14) and (15). Also, \(R\) is determined by the TF radius, Eq. (9). Note that, according to Eqs. (7) and (8), \(R_{TF}/\xi_d = (R_{TF}/l_\perp)^2/2 = (R_{TF}/l)^2/2\) when \(\nu = 1\). As \(0 \leq \tilde{r} \leq \tilde{R} = R/l_\perp\) for \(\nu = 1\), the (scaled) energy difference is independent of \(\omega_z\). While we thus only have to solve Eq. (14) for one specific value of \(\omega_z\) in order to assess the energetical stability against vortex dissociation, to verify the validity of our numerical code, we solved Eq. (14) for two different values of \(\omega_z\). Solving Eq. (14) in a harmonic trap is more time-consuming when compared to box traps (at the same lateral size), due to the boundary condition imposed on the wavefunction. For box traps, the boundary condition is simply \(\psi = 0\) when \(r = R\). However, for harmonic traps, there is no finite value of \(R_c\) where \(\psi = 0\) for \(r = R\). The TF radius equals \(R_c\) by definition only if we neglect the kinetic term in the GP equation. Therefore, if one sets \(\psi = 0\) at \(r = R_{a,c}\) where \(R_{a,c} \geq R_{TF}\) is some finite positive value in order to approximate the boundary when a harmonic trap is used with a corresponding TF radius \(R_{TF}\), near \(R_{a,c}\) the calculation burden increases in order to achieve \(\psi \approx 0\) at \(r = R_{a,c}\), even though \(\psi\) does not change significantly for \(r \geq R_{TF}\). Hence, to reduce the calculation time and memory cost, we set \(R = R_{TF} + l\) and performed calculations for \(R/\xi_d = 4, 8\).

Table I contains the \(R/\xi_d\), \(N\), \(\omega_z\) values which were investigated for the harmonic trap. First, fixing \(c_2 = c_0\), we changed \(N\) and obtained what is displayed in Fig. 3 from which we conclude that vortex dissociation is energetically more favorable in harmonic than in box traps. As discussed in the above, using Eqs. (14), (15), and (8), \(\Delta E_{H,S}\) is independent of the harmonic trap frequency \(\omega_z\) once \(\omega_z > 0\). To investigate whether \((c_2/c_0)_{cr}\) depends on the type of trap potential, we fixed \(R/\xi_d = 4\) and changed \(c_2\) while fixing \(c_0\) (see Fig. 4). Again, Fig. 4 states that spin-spin coupling driven vortex dissociation is energetically more likely in harmonic traps when compared to box traps, the critical ratio \((c_2/c_0)_{cr}\) being smaller in the box trap. By plotting \(\Delta E_{H,S}\) in a harmonic trap, Fig. 5, we find that \(\Delta E_{H,S}\) has double peaks, as in the box trap, Fig. 2.

Taking into account the harmonic trap energy, the latter is for two HQVs smaller than with a SQV at the center; their difference however decreases when \(c_2 \to \infty\). Hence, for the same \(R/\xi_d\), the critical \((c_2/c_0)_{cr}\) in harmonic traps is larger than in box traps, as Table II demonstrates.

![Figure 3](image_url)  
**FIG. 3.** Scaled energy difference \(\Delta E_{H,S}\) as a function of \(R/\xi_d\) for \(D/\xi_d = 1\), for box and harmonic traps. Here, \(c_2 = c_0\). Values of \(R/\xi_d\) and \(N\) are in Table I. We conclude that, relative to the box trap potential, the harmonic trap potential facilitates dissociation.

**TABLE II.** The critical \((c_2/c_0)_{cr}\) for box and harmonic traps.

| Trap Type | \(R/\xi_d\) | \(c_2/c_0)_{cr}\) | \(R/\xi_d\) | \(c_2/c_0)_{cr}\) |
|-----------|-------------|-----------------|-------------|-----------------|
| Box Trap  | 4           | 1.9             | 8           | 1.19            |
| Harmonic Trap | 4           | 2.3             | 8           | 1.38            |

**IV. CONCLUSION**

Using mean-field theory, we numerically obtained the critical value of the ratio of spin-spin and density-density couplings, \((c_2/c_0)_{cr}\), for SQV dissociation into two HQVs to take place in a trapped spin-one condensate. Vortex dissociation was demonstrated to be energetically disfavored when \(c_2/c_0 > (c_2/c_0)_{cr}\) given \(c_0 > 0\) and the system is in the AF phase. With a box trap potential, and hence in a relatively homogeneous situation, we obtained consistency with the results of [33]. Moreover, our results predict that the intervortex force between two oppositely charged HQVs is repulsive for \(c_2/c_0 < (c_2/c_0)_{cr}\). This, in particular, generally implies that it remains repulsive for \(c_2/c_0 < 0\). Furthermore, vortex dissociation was shown...
to be energetically more favorable in a harmonic than in a box trap, in the sense that the critical \( (c_2/c_0)_c \) in harmonically trapped gases is larger than in box traps. For harmonic traps, we have also shown that \( (c_2/c_0)_c \) does not depend on the trap frequency \( \omega_\perp \) in the plane, and that \( (c_2/c_0)_c \) increases as \( R/\xi_d \) decreases, implying that stronger confinement necessitates larger spin-spin interaction to suppress the dissociation process in smaller systems.

While current experiments on spinor gases (for an overview see, e.g., [37]) all operate at the untuned, atomically pre-given small values of \( |c_2/c_0| \), both in sodium \( (c_2 > 0) \) as well as in rubidium \( (c_2 < 0) \), our predictions for the critical values of \( c_2/c_0 \) can be experimentally verified by tuning couplings using the microwave and radio-frequency techniques suggested in various theoretical proposals [48–50].

Finally, our calculations provide a valuable benchmark for the accuracy of the numerically highly demanding solution of coupled spinor GP equations, and hence for their predictive power regarding the dynamics of topological defects in ultracold quantum gases. The latter is here represented by a sensitive prediction for the critical dissociation point for single-quantum vortices into half-quantum vortices for mesoscopic samples. In such a process, an intricate interplay of various (interaction and single-particle) terms in the energy functional becomes important, and mean-field theory is tested sensitively in the presence of many such competing terms.

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