Absence of the twisted superfluid state in a mean-field model of bosons on a honeycomb lattice

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Motivated by recent observations [Soltan-Panahi *et al.*, Nat. Phys. **8**, 71 (2012)], we study the stability of a Bose-Einstein condensate within a spin-dependent honeycomb lattice towards forming a "twisted superfluid" state. Our exhaustive numerical search fails to find this phase, pointing to possible non-mean-field physics.

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I. INTRODUCTION

A. Background

Recently Soltan-Panahi *et al.* found evidence of a zero quasimomentum "twisted superfluid" state of a two-component Bose-Einstein condensate (BEC) trapped in a spin-dependent honeycomb lattice [1]. A twisted superfluid is characterized by Bose-Einstein condensation into a state whose order parameter (a macroscopically occupied single particle wave function) has a spatially varying phase. The simplest example is condensation at finite momentum. Alternatively, in a non-Bravais lattice where the unit cell involves multiple sites, one can have a twisted superfluid at zero quasimomentum if the phase of the order parameter varies throughout the unit cell. We model the experiment of Soltan-Panahi *et al.* [1] with a mean-field Gross-Pitaevskii function. We find that the twisted superfluid state is absent within mean-field theory thus suggesting that the observations are due to non-mean-field effects.

Twisted superfluids are quite exotic; the phase twists of the order parameter are naturally associated with microscopic currents. Moreover, the present example involves spontaneous symmetry breaking, and provides a setting for studying phase-transition physics. Analogous physics can be found in magnetic systems [2] and in the excited states of lattice bosons [3,4].

B. Experimental evidence for a twisted superfluid

In their experiment [1], Soltan-Panahi *et al.* created a two-component BEC of ^{87}Rb atoms in a spin-dependent honeycomb lattice. Soltan-Panahi *et al.* find evidence for the twisted superfluid state in two cases: a BEC of ^{87}Rb atoms in the $|F=1,m_F=-1\rangle$ and $|F=1,m_F=1\rangle$ states and a BEC of ^{87}Rb atoms in the $|F=2,m_F=-2\rangle$ and $|F=1,m_F=-1\rangle$ states. In both of these cases, the two spin states form out-of-phase charge density waves in this spin-dependent lattice. In Fig. 1, we show a cartoon of the density of atoms in one of the two spin states. For the rest of this paper, we focus on the case where the two spin states are $|F=1,m_F=-1\rangle$ and $|F=1,m_F=1\rangle$.

The main experimental evidence for nontrivial phases of the superfluid order parameter comes from time-of-flight expansion, a technique where all trapping fields are removed and the atomic ensemble falls freely under gravity. Neglecting interactions [5], the long-time real space density profile is simply the initial density in momentum space. For the special case of a BEC, the momentum space density, n_k is the Fourier transform of the order parameter: $n_k=|\psi(\mathbf{k})|^2=|\int \exp(+i\mathbf{k}\cdot\mathbf{r})\psi(\mathbf{r})|^2$, where $\psi(\mathbf{r})$ is the order parameter of the BEC. As schematically illustrated in Fig. 2, if $\psi(\mathbf{r})$ is real, and has the symmetry of the honeycomb lattice, its Fourier transform (and consequently the time-of-flight pattern) is sixfold symmetric. This sixfold symmetry persists even if the densities on the two sublattices differ, forming a threefold symmetric charge density wave as illustrated in Fig. 1. Mathematically, this sixfold rotational symmetry of the time-of-flight pattern is a consequence of the point group symmetry of the lattice (C_{3v}) and the relation $\psi(-\mathbf{k})=\psi^*(\mathbf{k})$, which holds for real $\psi(\mathbf{r})$. Therefore, a time-of-flight pattern without inversion symmetry [$\psi(-\mathbf{k})\neq\psi^*(\mathbf{k})$] is direct evidence of a complex wave function (i.e., a twisted superfluid state). The experimentalists see exactly this signature.

From the time-of-flight images obtained in [1], a breakdown of the sixfold rotational symmetry in momentum space is observed for lattice depths V_{lat} ranging from about 1 to 4 E_{R}, where $E_{\text{R}}=\frac{\hbar^2}{2m\lambda_L^2}$, m is the mass of ^{87}Rb atoms, and V_{lat} is precisely defined by Eq. (6). Figure 2 illustrates this structure in which the amplitudes of the first order time-of-flight peaks (denoted by $|t|$ and $|z|$) have different values for this range of lattice depths. An important aspect of their experiment was that this rotational symmetry breaking arises only if both species of atoms are present. Moreover, the symmetry breaking was opposite for the two species (i.e., $\frac{|t_1|}{|z_1|}=\frac{|z_2|}{|t_2|}$). The order parameter O for the twisted superfluid state is given by

$$O=\left|\frac{|z|^2-|t|^2}{|z|^2+|t|^2}\right|. \tag{1}$$

By construction, O has a nonzero value in the twisted superfluid and is zero for a uniform condensate. Soltan-Panahi *et al.* measure this quantity.

The experimental evidence suggests that the order parameter is uniform on each of the triangular sublattices of the honeycomb lattice, but that there is a relative phase δ between them.

$$|z|^2=n_++n_-+2\sqrt{n_+n_-}\sin(\delta) \quad \text{and} \tag{2}$$

$$|t|^2=n_++n_--2\sqrt{n_+n_-}\sin(\delta), \tag{3}$$

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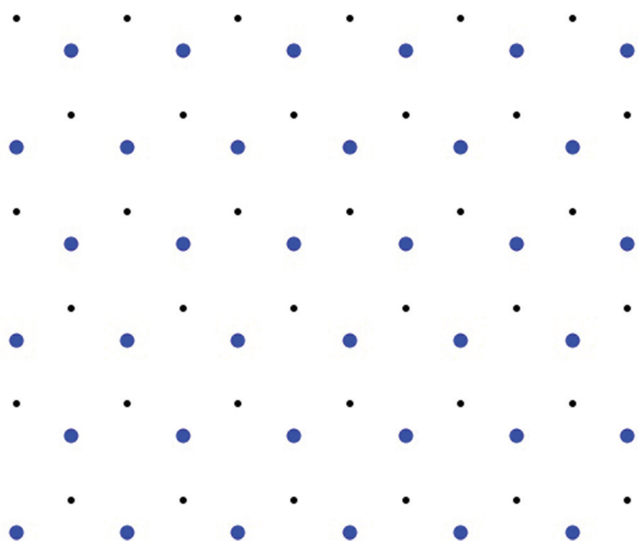

FIG. 1. (Color online) The density wave formed in a honeycomb lattice for the $m_F = 1$ atoms. The points represent lattice sites. Larger points indicate a site filled with more atoms. This pattern is periodically repeated. A complementary density wave is formed by $m_F = -1$ atoms. This density wave does not lead to a sixfold symmetry breaking in time-of-flight unless additional phases appear on the sites.

where n_+ and n_- denote the density of atoms on the two distinct sublattices. Thus, the order parameter is

$$O = \frac{2\sqrt{n_+ n_-}|\sin(\delta)|}{n_+ + n_-}. \tag{4}$$

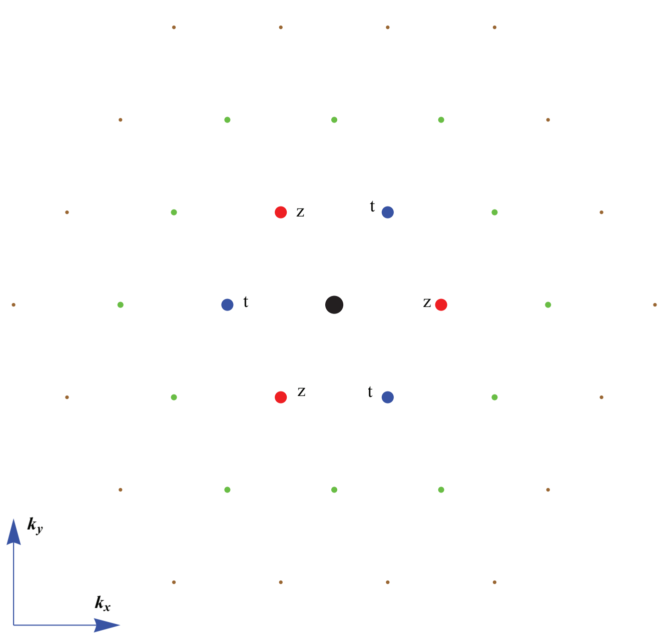

FIG. 2. (Color online) Schematic of the time-of-flight pattern for a superfluid in a 2D honeycomb lattice. Larger darker dots correspond to more particles with a given momentum. The complex numbers $|t|$ and $|z|$ represent the amplitudes of the Fourier transform of the condensate wave function at $k = (\frac{\pi}{a},0)$ and $k = (\frac{\sqrt{3}\pi}{2a},\frac{\pi}{2a})$ (see text). The twisted superfluid is described by $|t| \neq |z|$.

II. THE MODEL

Within a mean-field model, we will investigate the relative stability of twisted or ordinary superfluids. The energy of a two-component BEC, described by macroscopic wave functions ψ_1 and ψ_2 is

$$\begin{aligned} E_{3\mathrm{D}} = \int d^3\mathbf{r} \sum_{\sigma=1,2} \bigg[& \frac{\hbar^2}{2m}|\nabla\psi_\sigma(\mathbf{r})|^2 + V_\sigma(\mathbf{r})|\psi_\sigma(\mathbf{r})|^2 \\ & + \frac{U_{3\mathrm{D}}^\sigma}{2}|\psi_\sigma(\mathbf{r})|^4\bigg] + W_{3\mathrm{D}}|\psi_1(\mathbf{r})|^2|\psi_2(\mathbf{r})|^2 \\ & + V_{\mathrm{conf}}(\mathbf{r})[|\psi_1(\mathbf{r})|^2 + |\psi_2(\mathbf{r})|^2]. \end{aligned} \tag{5}$$

Here, $U_{3\mathrm{D}}^\sigma = \frac{4\pi\hbar^2 a_\sigma}{m}$ is the intraspecies interaction energy (a_σ is the intraspecies scattering length for species σ), while $W_{3\mathrm{D}} = \frac{4\pi\hbar^2 a_{12}}{m}$ is the interspecies interaction energy (a_{12} is the interspecies scattering length). As already mentioned in Sec. I B, we focus on the case in [1], where the states 1 (described by ψ_1) and 2 (described by ψ_2) are the $|F = 1, m_F = 1\rangle$ and $|F = 1, m_F = -1\rangle$ states of ^{87}Rb. For these two hyperfine states of ^{87}Rb atoms, $U_{3\mathrm{D}}^1$, $U_{3\mathrm{D}}^2$, and $W_{3\mathrm{D}}$ are almost equal ($a \approx 100a_0$ where a_0 is the Bohr radius). In principle, collisions can connect these hyperfine states to others (for example, $|F = 1, m_F = 0\rangle$). For the experimental parameters, these processes are off resonant and the two-component Bose gas model describes the physics.

In the experiment [1], the honeycomb lattice is generated by three lasers yielding a potential $V_i(\mathbf{r}) = V_{\mathrm{hex}}(\mathbf{r}) \pm \alpha B_{\mathrm{eff}}(\mathbf{r})$, where state 1 sees the sign "+" and state 2 sees the sign "−" (with $\alpha = 0.13$) and

$$\begin{aligned} V_{\mathrm{hex}}(\mathbf{r}) = 2V_{\mathrm{lat}}(&\cos[k_L\mathbf{b_1}\cdot x] + \cos[k_L\mathbf{b_2}\cdot\mathbf{x}] \\ &+ \cos[k_L\mathbf{b_3}\cdot\mathbf{x}]), \end{aligned} \tag{6}$$

$$\begin{aligned} B_{\mathrm{eff}}(\mathbf{r}) = 2\sqrt{3}V_{\mathrm{lat}}(&\sin[k_L\mathbf{b_1}\cdot\mathbf{x}] + \sin[k_L\mathbf{b_2}\cdot\mathbf{x}] \\ &+ \sin[k_L\mathbf{b_3}\cdot\mathbf{x}]), \end{aligned} \tag{7}$$

where $\mathbf{b_1} = -\frac{1}{2}\mathbf{e_x} - \frac{\sqrt{3}}{2}\mathbf{e_y}$; $\mathbf{b_2} = \mathbf{e_x}$; $\mathbf{b_3} = -\frac{1}{2}\mathbf{e_x} + \frac{\sqrt{3}}{2}\mathbf{e_y}$; and $k_L = 2\sqrt{3}\pi/\lambda_L$ (λ_L is the laser wavelength and is 830 nm for the experiment under discussion). With these considerations V_{lat} is the height of the barrier between neighboring sites. The difference between the maximum and minimum values of $V_{\mathrm{hex}}(\mathbf{r})$ is $8V_{\mathrm{lat}}$.

The experiment uses a separate set of lasers to provide strong confinement in the third dimension, $V_{\mathrm{conf}}(\mathbf{r})$:

$$V_{\mathrm{conf}}(\mathbf{r}) = V_{1\mathrm{D}}\cos\left[\frac{2\pi}{\lambda_{1\mathrm{D}}}z\right] \approx \frac{V_{1\mathrm{D}}}{2}\left(\frac{2\pi}{\lambda_{1\mathrm{D}}}\right)^2 z^2. \tag{8}$$

This potential restricts the dynamics to two dimensions and we may take the wave function of the BEC in the third direction to be constant and Gaussian. Then the energy can be written as

$$\begin{aligned} E_{2\mathrm{D}} = \int d^2\mathbf{r} \sum_{\sigma=1,2} \bigg[& -\frac{\hbar^2}{2m}\nabla^2\psi_\sigma(\mathbf{r}) + V_\sigma(\mathbf{r})|\psi_i(\mathbf{r})|^2 \\ & + \frac{U_{2\mathrm{D}}}{2}|\psi_\sigma(\mathbf{r})|^4\bigg] + W_{2\mathrm{D}}|\psi_1(\mathbf{r})|^2|\psi_2(\mathbf{r})|^2, \end{aligned} \tag{9}$$

where $U_{2D} = U_{3D}\sqrt{\frac{\sqrt{mV_{1D}}2\pi}{\lambda_{1D}h}}$ and $W_{2D} = W_{3D}\sqrt{\frac{\sqrt{mV_{1D}}2\pi}{\lambda_{1D}h}}$. In the experiment [1], $\lambda_{1D} = \lambda_L = 830$ nm and $V_{1D} = 8.8E_R$. For these parameters, the weakest lattice yielding a Mott state is $V_{lat} \approx 3.5E_R$ for two particles per unit cell within the Gutzwiller mean-field approximation [6].

We assume a form of $\psi_1(\mathbf{r})$ and $\psi_2(\mathbf{r})$ which is consistent with the time-of-flight measurements:

$$\psi_1(\mathbf{r}) = \sum_k \psi_1(\mathbf{k}) \exp(-i\mathbf{k}\cdot\mathbf{r}), \tag{10}$$

$$\psi_2(\mathbf{r}) = \sum_k \psi_2(\mathbf{k}) \exp(-i\mathbf{k}\cdot\mathbf{r}), \tag{11}$$

where $\mathbf{k}$ are the reciprocal lattice vectors of a honeycomb lattice. We insert this variational ansatz into Eq. (5) and minimize the energy with respect to the set of variational parameters $\psi_1(\mathbf{k})$ and $\psi_2(\mathbf{k})$. We find from our simulations that for all experimental parameters $\psi_1(\mathbf{k}) = \psi_2^*(\mathbf{k})$, where $\psi_2^*(\mathbf{k})$ is the complex conjugate of $\psi_2(\mathbf{k})$. This result is sensible and implies ψ_1 and ψ_2 are related by a lattice translation.

We perform the variational minimization in Fourier space rather than real space (where such minimization is usually done). This is equivalent to solving the Gross-Pitaevskii equation in real space within a single unit cell with periodic boundary conditions. Computationally, we find momentum space to be more efficient. Moreover, the experimental probes are all in momentum space. Similar approaches have been used by other authors [7–9].

III. METHOD

In k space, the energy, Eq. (9), becomes

$$\begin{aligned}\frac{E_{2D}}{E_R} = \sum_{\{\mathbf{k},\mathbf{k_1},\mathbf{k_2},\mathbf{k_3}\}\epsilon\overline{\mathcal{L}}} \sum_{i=1,2} \Big[& 3k^2\psi_i^*(\mathbf{k})\psi_i(\mathbf{k}) \\ & + V_i(\mathbf{k_1})\psi_i^*(\mathbf{k_2})\psi_i(\mathbf{k_2}-\mathbf{k_1}) \\ & + \frac{U}{2}\psi_i^*(\mathbf{k_1})\psi_i^*(\mathbf{k_2})\psi_i(\mathbf{k_3})\psi_i(\mathbf{k_1}+\mathbf{k_2}-\mathbf{k_3})\Big] \\ & + W\psi_1^*(\mathbf{k_1})\psi_1(\mathbf{k_2})\psi_2^*(\mathbf{k_3})\psi_2(\mathbf{k_1}+\mathbf{k_3}-\mathbf{k_2}),\end{aligned} \tag{12}$$

where $\overline{\mathcal{L}}$ stands for the reciprocal lattice, i.e., $\mathbf{k} = (a_1\mathbf{b_1} + a_2\mathbf{b_2})$, a_1 and a_2 being integers and $k = |\mathbf{k}|$. One can also generate this lattice from one of $\mathbf{b_1}$, $\mathbf{b_2}$, and $\mathbf{b_3}$, all explicitly given following Eq. (7). All energies (V_i, U, and W) are expressed in terms of E_R.

While we carried out unrestricted minimizations, our results are best illustrated by considering an ansatz where the low momentum physics is characterized by two complex numbers t and z. In particular, we take $\psi_1(\mathbf{k}) = t$ and $\psi_2(\mathbf{k}) = z$ for $\mathbf{k} = \{\mathbf{b_1},\mathbf{b_2},\mathbf{b_3}\}$ and $\psi_1(\mathbf{k}) = z$ and $\psi_2(\mathbf{k}) = t$ for $\mathbf{k} = \{-\mathbf{b_1}, -\mathbf{b_2}, -\mathbf{b_3}\}$. In terms of their real and imaginary parts, we write

$$t = t_r + it_i \tag{13}$$

and

$$z = z_r + iz_i. \tag{14}$$

As has been mentioned in Sec. I B, the order parameter for the twisted superfluid state is given by

$$O = \left|\frac{|z|^2 - |t|^2}{|z|^2 + |t|^2}\right|. \tag{15}$$

For our minimization, we restrict ourselves to $|\mathbf{k}| \leqslant 6$ giving us 159 complex variational parameters. We find that there are no differences if we use $|\mathbf{k}| \leqslant 4$ instead. Therefore, we believe our results faithfully reflect what would be found if an infinite number of Brillouin zones were included. We gain further confidence in the convergence of our results by noting that the fraction of population occupying the $|\mathbf{k}| = 4$ state when $U = 0.05E_R$ and $V_{lat} = 3.8E_R$ is about 0.0001%. It should also be noted that in the absence of interactions, at $V_{lat} = 4E_R$, the real space Wannier functions have width $\frac{1}{k_L}\sqrt{\frac{2}{3}}$ and the probability of having $|\mathbf{k}| \geqslant 2$ is less than 2%. Interactions tend to spread out the wave function, further reducing the occupation of high $|\mathbf{k}|$ states. In our simulations, we vary U in the range $0.03E_R$ to $0.2E_R$ corresponding to various strengths of the transverse confinement. For the experiment, $U \approx 0.05E_R$. We also vary α in the range 0.08–0.3, corresponding to varying amounts of detuning of the laser beams.

IV. RESULTS

We do not find any evidence for the existence of the twisted superfluid state despite an extensive search of the parameter space. Since Eq. (12) is a quartic form, it will in general have multiple minima and a number of other stationary points. The most grave concern with our results is that we might not have found the global minimum. To some extent, we can alleviate this concern by noting that the experiment finds a continuous symmetry breaking as a function of lattice depth. It therefore suffices to establish that our solution is a dynamically stable local minimum which is continuously connected to the symmetry-unbroken ground state at $V_{lat} = 0$.

A. Local energetic stability

We check whether whether we have found a true minimum by looking at the eigenvalues of the Hessian H defined by

$$H_{ij} = \frac{\partial^2 E}{\partial a_i \partial a_j}, \tag{16}$$

where a_i and a_j are real variational parameters [corresponding to the real and imaginary parts of $\psi(\mathbf{k})$]. We find that for all parameters, the eigenvalues of H are positive. This implies that we have at least found a local minimum. In Fig. 3, we plot the minimum eigenvalues of the Hessian for different values of the lattice depth (V_{lat}) at the illustrative interaction strength $U = 0.05E_R$ and $\alpha = 0.14$, for five particles (of each species) per unit cell.

We further illustrate the stability of our theory by doing two separate numerical experiments:

(a) Fix the ratio of z_r (Re[z]) to t_r (Re[t]) and vary the remaining variational parameters to find the energy minima. We find that the minimum of the energy occurs when $z_r : t_r = 1$ and there are no other local minima. The dotted curve shows this in Fig. 4.

(b) Fix the ratio of z_i (Im[z]) to t_i (Im[t]) and vary the remaining variational parameters to find the energy minima. We find that the minimum of the energy occurs when $z_i : t_i = 1$ and there are no other local minima. The solid curve shows this in Fig. 4.

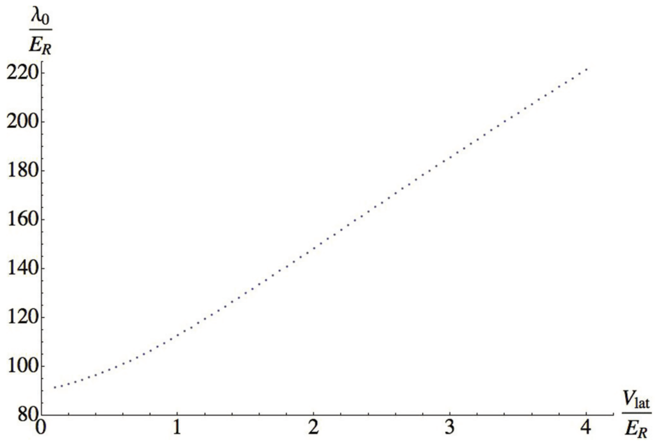

FIG. 3. Minimum eigenvalue of the Hessian, λ_0, in the normal superfluid phase plotted against the lattice depth V_{lat} (in units of E_{R}) when $U = 0.05E_{\text{R}}$ and five particles (of each species) are present per unit cell. All the eigenvalues of the Hessian are positive, thereby showing the stability of the normal phase. We conclude that there is no twisted superfluid state for these potential depths. This result is illustrative of all parameter ranges we explored.

We conclude that there is no second order phase transition within mean-field theory.

B. Local dynamic stability

We also check whether the minimum found is unstable against perturbations. This is done by looking at the Gross-Pitaevskii equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\partial E}{\partial\psi^*}. \tag{17}$$

This would imply

$$i\hbar\frac{\partial\delta a_j}{\partial t} = \frac{\delta E}{\delta a_j} \approx \sum_l \frac{\partial^2 E}{\partial a_j \partial a_l}\delta a_l. \tag{18}$$

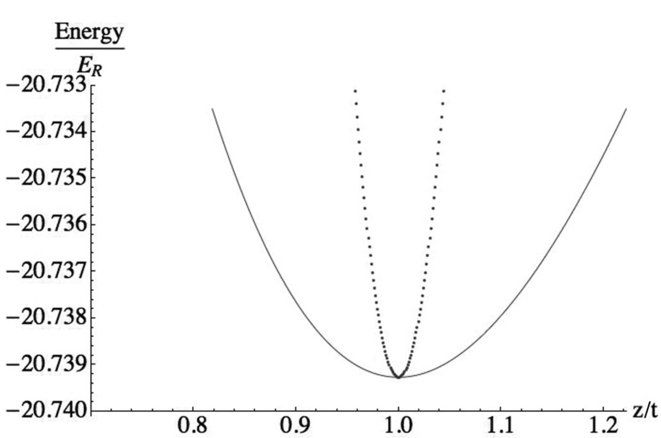

FIG. 4. (Color online) Slice through the energy landscape at $V_{\text{lat}} = 1.8E_{\text{R}}$ and $U = 0.05E_{\text{R}}$ and five particles (of each species) per unit cell. Dotted curve: The ratio Re[z]/Re[t]is varied and the energy is found by minimizing with respect to the other variational parameters. Solid curve: Same, but with varying Im[z]/Im[t]. We find that the overall energy minimum occurs when Re[z] = Re[t] and Im[z] = Im[t].

Taking the real and imaginary parts of both sides, we get the eigenvalue equations

$$\hbar\omega u = Mu, \tag{19}$$

where

$$M = \begin{bmatrix} \text{Re}[H] & -\text{Im}[H] \\ \text{Im}[H] & \text{Re}[H] \end{bmatrix}.$$

We look at the eigenvalues of this matrix, M. A complex eigenvalue would signify the presence of a mode which will grow with time, thus rendering this ground state unstable. We find that all the eigenvalues are real. Thus, the minimum that we have found is also dynamically stable. This is a generic feature of quantum systems: Energetic stability implies dynamic stability [10].

V. DISCUSSION

Given that our mean-field treatment of Eq. (5) fails to reproduce the experimental observations, we must now confront the question of what additional physics is needed to produce a twisted superfluid state. In this section, we present a tight-binding model which has a twisted superfluid ground state and discuss connections with our approach. Namely, consider a Hamiltonian

$$H = \sum_{\langle ij\rangle}(-t(\hat{a}^\dagger_{i\uparrow}\hat{a}_{j\uparrow} + \hat{a}^\dagger_{i\downarrow}\hat{a}_{i\downarrow}) + t_{\text{cf}}(\hat{a}^\dagger_{i\uparrow}\hat{a}^\dagger_{j\downarrow}\hat{a}_{j\uparrow}\hat{a}_{i\downarrow}) + \text{H.c.}). \tag{20}$$

Here, $a_{i\sigma}$ annihilates a particle labeled by the spin index σ on site i, and the sum is over all nearest-neighbor sites of a honeycomb lattice. The parameters t and t_{cf} represent single particle and counterflow hopping. We consider a mean-field ansatz where $\hat{a}_{j\sigma}$ is replaced by a c number, which can take one of two values, depending on which sublattice site j belongs to (see Fig. 1):

$$a_{j\uparrow} = \sqrt{n_+}\exp(-i\delta/2) \quad \text{sublattice } A \tag{21}$$

$$a_{j\uparrow} = \sqrt{n_-}\exp(+i\delta/2) \quad \text{sublattice } B \tag{22}$$

and

$$a_{j\downarrow} = \sqrt{n_-}\exp(+i\delta/2) \quad \text{sublattice } A \tag{23}$$

$$a_{j\downarrow} = \sqrt{n_+}\exp(-i\delta/2) \quad \text{sublattice } B. \tag{24}$$

A twisted superfluid corresponds to $\delta \neq 0$ and physically can be interpreted as a state where there are microscopic single particle currents, which are precisely balanced by microscopic counterflow currents. The mean-field energy per site is

$$E = [-12t\sqrt{n_+n_-}\cos(\delta) + 6t_{\text{cf}}n_+n_-\cos(2\delta)]. \tag{25}$$

The lowest energy state has $\delta \neq 0$ if

$$2t_{\text{cf}}(n_+n_-) > t\sqrt{n_+n_-}. \tag{26}$$

Our model in Eq. (5) contains terms of the same form as those in Eq. (25). For deep lattices [11],

$$t \sim |a|^{-3/2}\exp(-\pi\sqrt{V_{\text{lat}}/E_{\text{R}}}/2) \tag{27}$$

and

$$t_{\mathrm{cf}} \sim |a|^{-3} \exp(-\pi \sqrt{V_{\mathrm{lat}}/E_{\mathrm{R}}}), \tag{28}$$

where a is the distance between nearest neighbors. The exponential suppression of t_{cf} means that for any reasonable particle density, Eq. (26) is not satisfied. On the other hand, quantum fluctuations suppress single particle hopping more than counterflow [12–16], and a beyond mean field theory treatment of Eq. (5) could yield a twisted superfluid. Thus, the observations of Soltan-Panahi *et al.* [1] may be evidence of non-mean-field physics.

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