Diffraction catastrophes threaded by quantized vortex skeletons caused by atom-optical aberrations induced in trapped Bose-Einstein condensates

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We propose a nonlinear atom-optics experiment to create diffraction catastrophes threaded by quantized vortex skeletons in Bose–Einstein condensed matter waves. We show how atom-optical aberrations induced in trapped Bose–Einstein condensates evolve into specific caustic structures due to imperfect focusing. Vortex skeletons, whose cross-sections are staggered vortex lattices, are observed to nucleate inside the universal diffraction catastrophes. Our observations shed further light on the structure and dynamics of Bose-novae and suggest new kinds of flux lattices for cold atoms.

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Focusing is a generic phenomenon occurring in nature at all scales. Gravitational collapse leading to supernovae and black holes [1], sonoluminescence from imploding air bubbles [2], image formation on the retina of a human eye and Bose-novae of collapsing Bose–Einstein condensates [3–6] all involve focusing of light or matter into a small volume of space. Focusing is pivotal to many technological applications such as optical and electron microscopy, gravitational lensing and photography.

Natural focusing is rarely perfect, lens imperfections causing the well known optical aberrations such as astigmatism and coma. Imperfect lensing explodes a point focus, yielding extended caustics occupying a focal volume. The internal structure of such caustics can be described by the diffraction theory of aberrations [7] and catastrophe theory [8–11]. Remarkably, on closer inspection such caustics, which in ray optics correspond to infinite intensities, turn out to be perforated by a skeleton of quantized vortices and antivortices whose void cores define lines of strictly zero intensity [12]. In the spirit of particle–wave duality, Berry has put forth a conjecture of a caustic–vortex duality whereby the infinite intensities in the caustics are complementary to the zero intensity vortex cores [13].

The rich structure of quantized vortices which emerge inside caustics can be understood in terms of multi-wave interference phenomena where three [14] or more waves interfere destructively to produce lattices of quantized phase singularities [15–21]. Such nodal lines generically appear in systems described by complex valued wavefunctions. Optical vortices [22] and recently observed vortex knots [23] together with their matter wave cousins, electron vortices [24,27] and electron vortex loops [27], are examples of systems where coherent linear superposition of multiple wave trains yield nodal lines in complex wavefunctions. In addition to these linear systems, quantized vorticity is intimately connected with the phenomenon of superfluidity observed for example in He II [28] and Bose–Einstein condensed atomic gases [29]. In superfluids nonlinearities due to particle interactions are an inherent property of the system and the concept of a quantized vortex acquires perhaps its closest analog to the intuitive picture of a classical whirlpool.

Aberrated lensing, caustics, diffraction catastrophes and their connection to quantized vortices have been observed in light optics and more recently in electron matter waves [27]. Similar experiments focusing on matter wave lensing in superfluids are within reach of existing technology. However, a notable difference between photons or electrons that are used for microscopy and the condensates of cold atoms is that the latter are tuneably self-interacting and result in nonlinear atom-optics effects such as four-wave mixing [30].

Here we propose diffractive singular atom-optics experiments deploying the nonlinearity of the Bose–Einstein condensates to create and observe the internal structure...
of caustics and diffraction catastrophes which are punctured by quantized vortex skeletons. We show how nonlinear atom-atom interactions can induce drastic changes to the structure of such quantized vortex skeletons due to self-focusing. We consider a coherent ensemble of interacting Bose–Einstein condensed atoms, lensed by perturbations to the external potentials used for trapping the atoms. Such lens imperfections result in formation of condensate matter wave caustics \[31, 32\]. The scenario considered in this paper, where matter wave diffraction catastrophes spawn formation of quantized vortex skeletons in aberrated Bose–Einstein condensates, is illustrated by the schematic Fig. 1.}

We model the structure and dynamics of weakly interacting Bose–Einstein condensates using the Gross–Pitaevskii Hamiltonian \[34, 35\]
\[
H = \left( -\frac{\hbar^2 \nabla^2}{2m} + V(r,t) + g|\psi(r,t)|^2 \right),
\]
where \(\hbar\) is Planck’s constant, \(m\) is particle mass, \(g = 4\pi\hbar^2 a/m\) is the interaction coupling constant proportional to the s-wave scattering length \(a\), and \(V(r,t)\) is an external time-dependent potential used to confine and manipulate the atoms, explicitly accounting for the aberrating imperfections of the trapping potential. The strength and sign of the atom-atom interactions \(g\) can be routinely controlled using a Feshbach resonance technique \[33\].

Our numerical experiment begins with a Bose–Einstein condensate confined in a toroidal trap \(V(r,t = 0) = V_{osc}(r) + V_{LG}(r)\), where the harmonic oscillator potential \(V_{osc}(r) = m(\omega_{r}^2 r^2 + \omega_{z}^2 z^2)/2\) with \(\omega\) the Cartesian frequencies and the Mexican hat structure is achieved using a red-detuned Laguerre-Gauss laser mode to result in a potential \(V_{LG}(r) = -500(x^2+y^2)/\sigma^2 e^{-2(x^2+y^2)/\sigma^2 \hbar \omega}\), where \(\sigma = 20 a_{osc}\), with \(a_{osc} = \sqrt{\hbar/m\omega}\) the harmonic oscillator length \[36, 39\]. We consider cylindrically symmetric initial trap configurations \(\omega_{r} = \omega_{z} = \omega_{y}\) with \(\omega_y = 5 \omega_{r}\) and interaction strength \(g' = gN/\hbar \omega_{r} a_{osc}^3 = 5000\), where \(N\) is the number of particles in the condensate. In the ground state of this potential the condensate takes the shape of the usual Thomas–Fermi doughnut and the phase map \(S(r) = \arg(\psi(r,t))\) is spatially constant throughout the condensate.

The motivation for using such ring trapped condensates is to remove the high intensity of atoms from within the interior of the caustic structures, which would otherwise hinder the formation of vortices inside the diffraction catastrophes. Moreover, the stability of the caustic structures increases as the width of the toroid is reduced and in the limit of infinitely narrow condensate toroids the caustics approach propagation invariance. The form of our toroidal condensate is further motivated by recent experiments which utilized such a trapping geometry to study persistent currents in Bose–Einstein condensates \[37, 39\]. In the context of this work, such trapping potentials are aptly suited for creating and experimentally observing vortex skeletons, which demonstrably nucleate within the diffraction catastrophes of aberrated Bose–Einstein condensates.

Consider an externally applied potential of the form \(V_{lens}(r) = \sum_{n=-\infty}^{\infty} \sum_{m=0}^{\infty} \beta(n, m) Z_{n,m}^{r}(r)\) where \(\beta\) is a real number and \(Z_{n,m}^{r}(r)\) is a Zernike polynomial indexed by \((n, m)\) \[40\]. When applied for a short duration \(\Delta t\) (in comparison to other relevant time scales in the problem) this potential corresponds to the atom-optic analog of a thin lens. Each Zernike polynomial \(Z_{n,m}^{r}\) produces a different kind of lens aberration such as astigmatism or coma. The effect of such a potential pulse on a trapped ground state Bose–Einstein condensate is to imprint a complex phase to the macroscopic wavefunction describing the condensate leaving the particle density initially unchanged. Since the momentum of the atoms is proportional to the gradient of this phase, it also amounts to imparting a momentum distribution to the condensate, specified by the chosen aberration potential, see Fig 1(ii).

The matter wave lensing begins by switching off the external trapping potentials confining the ground state condensate. We thereafter consider two different experimental sequences: I apply the perturbing lens potential \(V_{lens}(r)\) to the interacting condensate for duration \(\Delta t\), after which a Feshbach resonance is used to tune the interaction strength to \(g' = 0\). Note that setting the lens perturbation equal the original trapping potential corresponds to a typical Bose-nova experiment. The condensate is then left to evolve ballistically in the time-of-flight
for a time $\tau$ before imaging the probability density distribution. In the second protocol II we tune close to $g' = 0$ first at the same time when the trapping potentials are turned off and after this apply the lens aberration for duration $\Delta t$ before imaging after an additional duration $\tau$ of time-of-flight. A third option would be to let the atoms interact throughout the experiment to observe how the nonlinear interactions cause bending of the atom trajectories for the whole duration of the time-of-flight, although the effect of these interactions would be rapidly washed away as the cloud is diluted during its free expansion. While experimentally straightforward, we do not pursue this third option further here.

For a non-interacting condensate the final state $\psi(r, t_f)$ of the condensate matter wave, after the ballistic time-of-flight evolution for the duration $\tau$, initially in a state $\psi(r, t_i)$, is obtained by integrating the Schrödinger equation $i\hbar \frac{\partial}{\partial t} \psi(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(r, t) + V(r) \psi(r, t)$. For linear systems the initial state $\psi(r, t_i)$ can be calculated by propagating the ground state $\psi(r, 0)$ by using the potential operator only. However, for interacting condensates the solution must be obtained by propagating the field using the full Hamiltonian including the self-interactions. Here we obtain the initial states $\psi(r, t_i)$ by solving the three-dimensional time-dependent Gross–Pitaevskii equation until the particle interactions and all trapping potentials are turned off. The Fourier transformed condensate wavefunction is multiplied by a free propagator and back transformed to real space to obtain the spatial condensate density corresponding to the experimentally measurable probability density of atoms.

Figure 2(a) shows the condensate density $|\psi(z = 0)|^2$ immediately after application of the astigmatic lens perturbation $V_{\text{lens}}(r) = 0.08(x^2 - y^2)\omega_{\perp}/a_{\text{osc}}^2 \propto r^2$ for the duration $\Delta t = 0.005$ and shows that the aberrating lens perturbation is sufficiently short that it has not affected the spatial particle density distribution. However, the phase of the wavefunction, shown for the $z$ plane in (b) and (f), and which determines the momentum distribution of the atoms, is drastically different depending on whether method II or I is used, respectively. This is because the nonlinear particle interactions cause intrinsic lensing or self-focusing, in addition to the externally applied lens potential. This nonlinear effect becomes readily observable in the far field images of the condensate density. Frames (c) and (g) display the particle probability density after $\tau\omega_{\perp} = 1.5$ and $\tau\omega_{\perp} = 0.275$ of time-of-flight showing how the respective momentum distributions in (b) and (f) are sources of different internal diffraction detail of the caustics. Frame (d) shows the full quantized vortex skeleton (white dotted lines) which supports the caustic structure, together with an isodensity surface illustrating the caustic flesh. The caustic body has been cut through with a contour plot and the corresponding caustic cross-section, which reveals the staggered lattice of quantized vortices and antivortices, is shown in (e). Movies showing the evolution of these caustics are in the Supplemental Material [41].

The “salmiakki” shaped caustics in Fig. 2 embody the doubly folded manifolds with four cusps in the corners of the caustic. Such flared rhombi are the telltale signature of astigmatic lensing. The Einstein Cross Gravitational Lens G2237 + 0305 and the images of collapsing Bose–Einstein condensates [1][10] are further examples of similar caustic shapes. The structure in Fig. 2(g) reveals that the combination of astigmatism and intrinsic nonlinear lensing produces similar images as an aberrated axicon [12]. Instead of more conventional harmonically trapped systems, we have focused on toroidal condensates to enhance vortex production inside the caustics. For comparison, we have included an example in the Supplemental Material of an astigmatic lensing of a simply connected Bose–Einstein condensate, and a coma aberrated hyperbolic umbilic diffraction catastrophe in a ring-trapped condensate.

Figures 3(a)-(f) show a through focus series of images of time-of-flight showing how the respective momentum densities after $\tau\omega_{\perp} = 0.05$ and shows that the aberrat-
ages of a condensate particle density obtained after varying time of ballistic expansion after the application of a $\Delta t \omega_\perp = 0.005$ long aberrating trefoil lens perturbation of the form $V_{\text{lens}}(r) = 0.01(x^3 - 3xy^2) \hbar \omega_\perp / a_{\text{osc}}^3 \propto Z_3^3(r)$ using method II, which results in the elliptic umbilic diffraction catastrophe. Frames (g) and (h) show the condensate density after $\tau \omega_\perp = 0.04$ and $\tau \omega_\perp = 1.0$ of ballistic expansion, respectively, when method I is used. Again, the nonlinear particle interactions induce enriched quantized vortex skeletons inside the diffraction catastrophes. Frame (j) shows the phase map corresponding to central region of the frame (b). Movies showing the evolution of the caustics are in the Supplemental Material [11].

In the case of five-fold symmetric lens aberration, pentafoil snowflake patterns shown in Fig. 4 emerge. In this case $V_{\text{lens}}(r) = 0.0001(5x^4y - 10x^2y^3 + y^5) \hbar \omega_\perp / a_{\text{osc}}^5 \propto Z_5^5(r)$ and $\Delta \omega_\perp = 0.0075$. Frames (a)-(d) are obtained using method II and the frames (e) and (f) are for the case I. It is straightforward to extend these results to include higher order aberrations which yield a hierarchy of ever more complex diffraction detail and vortex skeletons. Irregular focusing can be modeled by considering a stochastic lens aberration obtained by randomly choosing the coefficients $\beta(n, m)$ of the lens polynomials. Alternatively, a speckled lens aberration can be produced for example by Fourier transforming a band limited white noise random potential. The vortex skeleton structures which emerge due to such stochastic focusing bear similarity to the vortex networks generated by the Kosterlitz–Thouless and Kibble–Zurek mechanisms. In rapidly rotating condensates melting of vortex lattices is predicted en route to quantum turbulence. The regular crystalline vortex order which emerge in diffraction catastrophes of linear systems can be melted by the nonlinearity due to particle interactions [19]. In sufficiently dilute systems, similar melting of vortex skeletons may occur also due to quantum fluctuations.

In conclusion, we have presented a nonlinear atom-optics protocol to create and observe aberration induced diffraction catastrophes and the associated skeletons of quantized vortices using cold atom experiments. In such experiments, imaging the internal structure of these caustics would benefit from a resolution boost obtained by adding a defocus (antitrapping) to the atom-optic lens perturbation to increase the physical size of the diffraction catastrophes. The matter wave diffraction catastrophes are generic and can also be generated using fermions or molecules. In spinor condensates the caustic vortex skeletons will be composed of fractional vortices and may result in non-Abelian vortex networks [20, 43, 44]. It should also be possible to use the method of atom-optic lens aberrations and focussing to nucleate vortex rings [27] and knotted matter wave vortices.

Interpreting the collapse of Bose–Einstein condensates in Bose-nova experiments in the context of aberrated matter wave lensing, the observed salmiakki shapes [4–6] are suggestive of caustic diffraction catastrophes caused by the quadrupole anisotropy in the trapping potentials, which in terms of lens aberrations correspond to astigmatism, see also Supplemental Material [11]. In light of this, we note that it is difficult to distinguish between the contributions arising from external lensing due to trap anisotropy and possible internal lensing due to dipolar interactions to the observed images [4–6], because both of these contributions produce the same lens aberration ($Z_2^2$ astigmatism). Furthermore, the generic telltale astigmatic caustic shape formed by rays of atoms emerges due to quadrupolar trap anisotropy even in the absence of any particle interactions.

Replacing the diffraction catastrophes of matter waves by those made of light opens the possibility to create exotic and steep walled light shift potentials for cold atoms since the tuneable diffraction catastrophes of the laser field can be made static in the reference frame of the trapped ground state condensate. Bragg scattering with Laguerre–Gauss beams have been used for transferring orbital angular momentum, or the phase of the photon field, to Bose–Einstein condensates [45]. Other kinds of spatial gradients of light-induced momentum have also been used to create artificial gauge fields for ultracold atoms [46, 47]. Photon fields sourced from aberration induced diffraction catastrophes may enable the creation of novel optical flux lattices for ultracold atoms [48, 50] and the resulting staggered vortex lattice states could be useful for studies of quantum turbulence and might lead to the realization of new emergent topological quantum states.
