# Appendix E: Lagrangian variational techniques in paraxial vortex dynamics

In this Appendix, attention is paid to the evolution of an optical vortex solution of the NLS equation. For simplicity, three cases of increasing complexity are considered which consist of a broad Gaussian background beam with (a) no singularity, (b) an on-axis singularity and (c) an off-axis singularity. A Lagrangian method is employed since exact analytical vortex solutions of the (2+1)D governing equation, where the diffraction operator captures two transverse dimensions, are unknown. Such variational descriptions are mathematically simpler and more physically transparent than other techniques, such as 'matched asymptotics' [Y. S. Kivshar *et al.*, Opt. Commun. **152**, 198 (1998); B. Luther-Davies *et al.*, J. Opt. Soc. Am. B **14**, 3045 (1997); J. Christou *et al*., Opt. Lett. **15**, 1649 (1996)].

The NLS vortex problem has previously been analysed by Syed [K. Syed, MSc.thesis "*Optical vorticies and spatial dark solitons in passive nonlinear media*," University of Strathclyde (1991)]. However, in one particular case, the published Euler equations of motion contain a small error. The motivation behind this subsequent analysis is thus to verify the validity of the equations of motion for cases (a) and (b), reported by McDonald *et al.* [G. S. McDonald, K. S. Syed and W. J. Firth, Opt. Commun. **94**, 496 (1992)], and to derive the correct coupled system for case (c).

## E1. Variational Framework

The NLS equation may be written as

$$i\frac{\partial F}{\partial \zeta}+\frac{\alpha}{2}\nabla_{\perp}^{2}F+\sigma\left|F\right|^{2}F=0\,, \tag{E1}$$

where $\nabla_\perp^2$ is the two-dimensional transverse Laplacian, $\alpha$ determines the scale of the transverse coordinates and $\sigma = \pm 1$ flags a focusing/defocusing Kerr non-linearity. Equation (E1) can be regarded as the Euler-Lagrange equation of motion for a Lagrangian density *L*, where

$$L\{F\} = \frac{i}{2}\left( F^* \frac{\partial F}{\partial \zeta} - F \frac{\partial F^*}{\partial \zeta} \right) - \frac{\alpha}{2}\left|\underline{\nabla}_\perp F\right|^2 + \frac{\sigma}{2}\left|F\right|^4 \tag{E2}$$

satisfies the field equation $\partial L / \partial F^* = 0$, or

$$\frac{\partial L}{\partial F^*} - \underline{\nabla}_\perp \cdot \frac{\partial L}{\partial\left(\underline{\nabla}_\perp F^*\right)} - \frac{\partial}{\partial \zeta}\frac{\partial L}{\partial\left(\partial_\zeta F^*\right)} = 0 . \tag{E3}$$

To proceed with the analysis, an ansatz is chosen for the functional form of the vortex field *F*, which is defined by a set of variational parameters $\{\beta\}$. The total Lagrangian $\ell$ is then obtained by integrating $L\{F\}$ over the transverse plane $\Omega$:

$$\ell \equiv \iint_\Omega d^2\mathbf{x}_\perp \; L\{F\} , \tag{E4}$$

where $\mathbf{x}_\perp$ is a suitable set of transverse coordinates. From this quantity, the longitudinal evolution of the parameter set $\{\beta\}$ can be calculated with recourse to the standard Euler equations of motion:

$$\frac{\delta \ell}{\delta \beta} = 0 , \qquad \text{or} \qquad \frac{\partial \ell}{\partial \beta} - \frac{d}{d\zeta}\frac{\partial \ell}{\partial\left(d\beta/d\zeta\right)} = 0 . \tag{E5}$$

In practice, it is sensible to adopt a coordinate system most appropriate for studying vortex dynamics, that is, one with obvious rotational symmetry in the transverse plane. In this case, we use plane-polar coordinates $(r, \theta)$ and Eq. (E4) for the system Lagrangian becomes

$$\ell = \int_0^{+\infty}\int_0^{2\pi} drd\theta \; rL\{F\} . \tag{E6}$$

## E2. GAUSSIAN BEAM

In this case, the ansatz assumes a particularly simple form:

$$F\left(\mathbf{x}_\perp,\zeta\right)=F_0\left(\zeta\right)\exp\left[-\gamma\left(\zeta\right)r^2\right], \quad \text{(E7)}$$

where $F_0$ and $\gamma$ are the variational parameters of the problem, and are potentially complex functions of $\zeta$. They are rewritten explicitly in terms of their real and imaginary parts,

$$F_0\left(\zeta\right)=F_R\left(\zeta\right)+iF_I\left(\zeta\right), \quad \text{(E8a)}$$

$$\gamma\left(\zeta\right)=\gamma_R\left(\zeta\right)+i\gamma_I\left(\zeta\right). \quad \text{(E8b)}$$

In this case, the rotational symmetry means that the transverse *gradient* operator is $\underline{\nabla}_\perp=\hat{\mathbf{r}}\partial_r$. By substituting Eqs. (E8) into Eq. (E6), the Lagrangian is found to be

$$\ell=\frac{\pi}{2}\left[\frac{1}{\gamma_R}\left(F_I\frac{dF_R}{d\zeta}-F_R\frac{dF_I}{d\zeta}\right)+\frac{1}{2\gamma_R^2}\left|F_0\right|^2\frac{d\gamma_I}{d\zeta}-\alpha\left(1+\frac{\gamma_I^2}{\gamma_R^2}\right)\left|F_0\right|^2+\frac{\sigma}{4\gamma_R}\left|F_0\right|^4\right], \quad \text{(E9)}$$

where $\left|F_0\right|^2=F_R^2+F_I^2$. Variation with respect to $\gamma_I$, $\gamma_R$, $F_I$ and $F_R$, respectively, yields the set of equations,

$$\frac{d}{d\zeta}\left|F_0\right|=-2\alpha\gamma_I\left|F_0\right|+\frac{\left|F_0\right|}{\gamma_R}\frac{d\gamma_R}{d\zeta}, \quad \text{(E10a)}$$

$$\gamma_R\left(F_I\frac{dF_R}{d\zeta}-F_R\frac{dF_I}{d\zeta}\right)+\left|F_0\right|^2\frac{d\gamma_I}{d\zeta}-2\alpha\gamma_I^2\left|F_0\right|^2+\frac{\sigma}{4}\gamma_R\left|F_0\right|^4=0, \quad \text{(E10b)}$$

$$\frac{2}{\gamma_R}\frac{dF_R}{d\zeta}+\frac{F_I}{\gamma_R^2}\frac{d\gamma_I}{d\zeta}-\frac{F_R}{\gamma_R^2}\frac{d\gamma_R}{d\zeta}-2\alpha\left(1+\frac{\gamma_I^2}{\gamma_R^2}\right)F_I+\frac{\sigma}{\gamma_R}\left(F_R^2+F_I^2\right)F_I=0, \quad \text{(E10c)}$$

$$-\frac{2}{\gamma_R}\frac{dF_I}{d\zeta}+\frac{F_R}{\gamma_R^2}\frac{d\gamma_I}{d\zeta}+\frac{F_I}{\gamma_R^2}\frac{d\gamma_R}{d\zeta}-2\alpha\left(1+\frac{\gamma_I^2}{\gamma_R^2}\right)F_R+\frac{\sigma}{\gamma_R}\left(F_R^2+F_I^2\right)F_R=0. \quad \text{(E10d)}$$

This system can be solved to yield three relatively simple equations of motion for the amplitude, waist and phase of the propagating spatial beam:

$$\frac{d|F_0|}{d\zeta} = 2\alpha\gamma_I |F_0|, \tag{E11a}$$

$$\frac{d\gamma_R}{d\zeta} = 4\alpha\gamma_I\gamma_R, \tag{E11b}$$

$$\frac{d\gamma_I}{d\zeta} = -2\alpha\left(\gamma_R^2 - \gamma_I^2\right) + \frac{\sigma}{2}\gamma_R |F_0|^2. \tag{E11c}$$

## E3. Gaussian Beam with On-Axis Phase Singularity

In this case, the beam has a seed at the origin, so that the vortex field may be described by

$$F(\mathbf{x}_\perp, \zeta) = F_0(\zeta)(\xi + i\eta)\exp\left[-\gamma(\zeta) r^2\right]. \tag{E12}$$

Following the same method, the Lagrangian is found to be

$$\ell = \frac{\pi}{2}\left[\frac{1}{2\gamma_R^2}\left(F_I \frac{dF_R}{d\zeta} - F_R \frac{dF_I}{d\zeta}\right) + \frac{1}{2\gamma_R^3}|F_0|^2 \frac{d\gamma_I}{d\zeta} - \frac{\alpha|F_0|^2}{\gamma_R}\left(1 + \frac{\gamma_I^2}{\gamma_R^2}\right) + \frac{\sigma}{\gamma_R^3}\frac{|F_0|^4}{32}\right]. \tag{E13}$$

The variational procedure can then be carried out, leading to the equations

$$\frac{d|F_0|}{d\zeta} = -2\alpha\gamma_I |F_0| + \frac{3}{2\gamma_R}|F_0|\frac{d\gamma_R}{d\zeta}, \tag{E14a}$$

$$\gamma_R\left(F_I \frac{dF_R}{d\zeta} - F_R \frac{dF_I}{d\zeta}\right) - \alpha\left(\gamma_R^2 + \gamma_I^2\right)|F_0|^2 - 2\alpha\gamma_I^2 |F_0|^2 + \frac{3}{2}|F_0|^2 \frac{d\gamma_I}{d\zeta} + \frac{3\sigma}{32}|F_0|^4 = 0, \tag{E14b}$$

$$\frac{1}{\gamma_R^2}\frac{dF_R}{d\zeta} + \frac{1}{\gamma_R^3}\left(F_I \frac{d\gamma_I}{d\zeta} - F_R \frac{d\gamma_R}{d\zeta}\right) + \frac{2\alpha}{\gamma_R}F_I\left(1 + \frac{\gamma_I^2}{\gamma_R^2}\right) - \frac{\sigma}{8\gamma_R^3}|F_0|^2 F_I = 0, \tag{E14c}$$

$$-\frac{1}{\gamma_R^2}\frac{dF_I}{d\zeta} + \frac{1}{\gamma_R^3}\left(F_R \frac{d\gamma_I}{d\zeta} + F_I \frac{d\gamma_R}{d\zeta}\right) - \frac{2\alpha}{\gamma_R}F_R\left(1 + \frac{\gamma_I^2}{\gamma_R^2}\right) + \frac{\sigma}{8\gamma_R^3}|F_0|^2 F_R = 0. \tag{E14d}$$

Again, the system can be simplified, and equations of motion derived for the beam amplitude, waist and phase:

$$\frac{d|F_0|}{d\zeta} = 4\alpha\gamma_I |F_0|, \tag{E15a}$$

$$\frac{d\gamma_R}{d\zeta} = 4\alpha\gamma_I\gamma_R, \tag{E15b}$$

$$\frac{d\gamma_I}{d\zeta} = -2\alpha\left(\gamma_R^2 - \gamma_I^2\right) + \frac{\sigma}{16}|F_0|^2. \tag{E15c}$$

These results can be generalized to the case of a vortex with an arbitrary topological charge. By recasting ansatz (13) into the form

$$F\left(\mathbf{x}_\perp,\zeta\right) = F_0\left(\zeta\right) r \exp\left[-\gamma\left(\zeta\right) r^2\right] \exp\left(im\theta\right),$$

where $m = \pm1, \pm2, \ldots$ labels the vortex charge, and repeating the analysis with the transverse diffraction operator expressed as $\underline{\nabla}_\perp = \hat{\mathbf{r}}\partial_r + \hat{\mathbf{e}}_\theta r^{-1}\partial_\theta$, variational equations (E15a) and (E15b) are recovered. The topological charge *m* appears explicitly only as a coefficient in the phase equation, whereby Eq. (E15c) is replaced by

$$\frac{d\gamma_I}{d\zeta} = -2\alpha\left(\frac{1+m^2}{2}\gamma_R^2 - \gamma_I^2\right) + \frac{\sigma}{16}|F_0|^2. \tag{E15d}$$

## E4. GAUSSIAN BEAM WITH OFF-AXIS PHASE SINGULARITY

In this case, the ansatz has the notable property of symmetry-breaking in the azimuthal coordinate $\theta$, where

$$F\left(\mathbf{x}_\perp,\zeta\right) = F_0\left(\zeta\right) \exp\left[-\gamma\left(\zeta\right) r^2\right]\left[r\exp\left(i\theta\right) - r_0\exp\left(i\phi\right)\right]. \tag{E16}$$

The phase singularity is located at a position $\mathbf{x}_\perp^0 = \left(\xi_0, \eta_0\right) \equiv \left(r_0, \phi\right)$ in the complex plane, where these two parameters are to be treated as additional generalized coordinates. Substitution of Eq. (E16) into Eq. (E6) yields the Lagrangian,

$$\ell = \frac{\pi}{2}\left[\left(\frac{1}{2\gamma_R^2} + \frac{r_0^2}{\gamma_R}\right)\left(F_I \frac{dF_R}{d\zeta} - F_R \frac{dF_I}{d\zeta}\right) + \frac{|F_0|^2}{2}\left(\frac{1}{\gamma_R^3} + \frac{r_0^2}{\gamma_R^2}\right)\frac{d\gamma_I}{d\zeta} - \frac{r_0^2|F_0|^2}{\gamma_R}\frac{d\varphi}{d\zeta}\right.$$
$$\left. - \alpha|F_0|^2\left(r_0^2 + \frac{1}{\gamma_R} + r_0^2\frac{\gamma_I^2}{\gamma_R^2} + \frac{\gamma_I^2}{\gamma_R^3}\right) + \sigma|F_0|^4\left(\frac{1}{32\gamma_R^3} + \frac{r_0^2}{4\gamma_R^2} + \frac{r_0^4}{4\gamma_R}\right)\right]. \tag{E17}$$

In this example, there are six variational parameters, rather than the four of the previous two cases. The corresponding equations of motion are found to be

$$\frac{d}{d\zeta}\frac{r_0^2|F_0|^2}{\gamma_R} = 0\,, \tag{E18a}$$

$$\frac{2r_0}{\gamma_R}\left(F_I\frac{dF_R}{d\zeta} - F_R\frac{dF_I}{d\zeta}\right) + \frac{r_0}{\gamma_R^2}|F_0|^2\frac{d\gamma_I}{d\zeta} - \frac{2r_0}{\gamma_R}|F_0|^2\frac{d\phi}{d\zeta}$$
$$- 2\alpha r_0|F_0|^2\left(1 + \frac{\gamma_I^2}{\gamma_R^2}\right) + \sigma|F_0|^4\left(\frac{r_0^3}{\gamma_R} + \frac{r_0}{2\gamma_R^2}\right) = 0, \tag{E18b}$$

$$2\alpha|F_0|^2\left(\frac{r_0^2}{\gamma_R^2} + \frac{1}{\gamma_R^3}\right)\gamma_I + \frac{|F_0|}{\gamma_R^3}\frac{d|F_0|}{d\zeta} - \frac{|F_0|^2}{2\gamma_R^3}\left(r_0^2 + \frac{3}{\gamma_R}\right)\frac{d\gamma_R}{d\zeta} = 0, \tag{E18c}$$

$$\left(\frac{1}{\gamma_R^3} + \frac{r_0^2}{\gamma_R^2}\right)\left(F_I\frac{dF_R}{d\zeta} - F_R\frac{dF_I}{d\zeta}\right) - \frac{r_0^2|F_0|^2}{\gamma_R^2}\frac{d\phi}{d\zeta} + \frac{|F_0|^2}{2}\left(\frac{3}{\gamma_R^4} + \frac{2r_0^2}{\gamma_R^3}\right)\frac{d\gamma_I}{d\zeta}$$
$$- \alpha|F_0|^2\left(\frac{1}{\gamma_R^2} + 2r_0^2\frac{\gamma_I^2}{\gamma_R^3} + 3\frac{\gamma_I^2}{\gamma_R^4}\right) - \sigma|F_0|^4\left(\frac{3}{32\gamma_R^4} + \frac{r_0^2}{2\gamma_R^3} + \frac{r_0^4}{4\gamma_R^2}\right) = 0, \tag{E18d}$$

$$\left(\frac{1}{\gamma_R^2} + \frac{2r_0^2}{\gamma_R}\right)\frac{dF_R}{d\zeta} + F_I\left(\frac{1}{\gamma_R^3} + \frac{r_0^2}{\gamma_R^2}\right)\frac{d\gamma_I}{d\zeta} - \frac{2r_0^2F_I}{\gamma_R}\frac{d\phi}{d\zeta} - \frac{F_R}{\gamma_R^3}\frac{d\gamma_R}{d\zeta} - \frac{2F_Rr_0^2}{\gamma_R|F_0|}\frac{d|F_0|}{d\zeta}$$
$$- 2\alpha F_I\left(r_0^2 + \frac{1}{\gamma_R} + r_0^2\frac{\gamma_I^2}{\gamma_R^2} + \frac{\gamma_I^2}{\gamma_R^3}\right) + \sigma|F_0|^2 F_I\left(\frac{1}{8\gamma_R^3} + \frac{r_0^2}{\gamma_R^2} + \frac{r_0^4}{\gamma_R}\right) = 0, \tag{E18e}$$

$$-\left(\frac{1}{\gamma_R^2} + \frac{2r_0^2}{\gamma_R}\right)\frac{dF_I}{d\zeta} + F_R\left(\frac{1}{\gamma_R^3} + \frac{r_0^2}{\gamma_R^2}\right)\frac{d\gamma_I}{d\zeta} - \frac{2r_0^2F_R}{\gamma_R}\frac{d\phi}{d\zeta} + \frac{F_I}{\gamma_R^3}\frac{d\gamma_R}{d\zeta} + \frac{2F_Rr_0^2}{\gamma_R|F_0|}\frac{d|F_0|}{d\zeta}$$
$$- 2\alpha F_R\left(r_0^2 + \frac{1}{\gamma_R} + r_0^2\frac{\gamma_I^2}{\gamma_R^2} + \frac{\gamma_I^2}{\gamma_R^3}\right) + \sigma|F_0|^2 F_R\left(\frac{1}{8\gamma_R^3} + \frac{r_0^2}{\gamma_R^2} + \frac{r_0^4}{\gamma_R}\right) = 0. \tag{E18f}$$

The variational equations of motion (E18) demonstrate a much greater complexity than in the previous two cases. The system captures the effect of vortex drift, whereby an off-axis phase singularity orbits the beam centre throughout propagation. Equations (E18) can still be solved, yielding

$$\frac{d|F_0|}{d\zeta} = 4\alpha\gamma_I |F_0|, \tag{E19a}$$

$$\frac{d\gamma_R}{d\zeta} = 4\alpha\gamma_I\gamma_R, \tag{E19b}$$

$$\frac{d\gamma_I}{d\zeta} = -2\alpha\left(\gamma_R^2 - \gamma_I^2\right) + \frac{\sigma|F_0|^2}{2}\left[\gamma_R r_0^2 + \frac{1}{8\left(1+\gamma_R r_0^2\right)}\right], \tag{E19c}$$

$$\frac{d\phi}{d\zeta} = 2\alpha\gamma_R + \frac{\eta}{2}|F_0|^2\left[\frac{1}{4\gamma_R} - \frac{r_0^2}{2} - \frac{1}{8\gamma_R\left(1+\gamma_R r_0^2\right)}\right]. \tag{E19d}$$

It can be seen that inclusion of the additional generalized coordinates $\mathbf{x}_\perp^0 = \left(r_0, \phi\right)$, denoting the location of the phase singularity in plane-polar coordinates, leads to an additional conservation law for the system, Eq. (E18a). Equation (E19d) is a corrected version of Eq. (11) published in by McDonald *et al.*. It contains two sign changes in the square parenthesis, the middle factor of $r_0^2/2$ replaces the published factor of $\gamma_R r_0^2/2$, and there is an additional factor of $\gamma_R$ in the denominator of the final term.

## E5. CONCLUSIONS

The evolution of a phase singularity, seeded on a Gaussian beam, has been investigated analytically through a straightforward application of the principle of least action. Three physically distinct regimes have been examined, where there is initially no vortex (e.g. a purely Gaussian beam), a central singularity, then an off-centre singularity. As the complexity of the problem increases, the equations of motion for the beam's amplitude and waist remain unchanged. However, the equation for the phase becomes more complicated, and this influences the other parameters of the system via non-linear coupling.

The variational analysis presented here captures the phenomenon of vortex drift. The breaking of rotational symmetry by an off-centre singularity leads to net forces in the transverse plane (related to transverse gradients of the intensity) that cause the singularity to circulate around the beam centre (intensity maximum). This phenomenon is facilitated by the inclusion of a pair of additional generalized coordinates (the location of the singularity in the transverse plane), which leads ultimately to a new conservation law, Eq. (E18d), not seen with the previous cases where azimuthal symmetry is not violated.