High precision solutions to quantized vortices within Gross–Pitaevskii equation

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Abstract
The dynamics of vortices in Bose–Einstein condensates of dilute cold atoms can be well formulated by Gross–Pitaevskii equation. To better understand the properties of vortices, a systematic method to solve the nonlinear differential equation for the vortex to very high precision is proposed. Through two-point Padé approximants, these solutions are presented in terms of simple rational functions, which can be used in the simulation of vortex dynamics. The precision of the solutions is sensitive to the connecting parameter and the truncation orders. It can be improved significantly with a reasonable extension in the order of rational functions. The errors of the solutions and the limitation of two-point Padé approximants are discussed. This investigation may shed light on the exact solution to the nonlinear vortex equation.

Keywords: quantum vortex, Gross–Pitaevskii equation, two-point Padé approximants

(Some figures may appear in colour only in the online journal)

1. Introduction

Vortices are strongly nonlinear excitations in superfluids, which are quantized as topologic defects from the long range quantum phase coherence [1–3]. The formation, stability and dynamical properties of vortices have been intensively studied experimentally [4–8] and theoretically [9, 10]. Vortices play important roles not only in many-body quantum systems, but also in dark matter [11–13] and the phase transition of the early universe [14–17]. The structure of nonlinear dynamics for vortices is in connection with the gravitational field equation for the metric of black holes, which makes it possible to study the Penrose process of rotating black holes in laboratories [18, 19]. Vortices are also necessary degrees of freedom in turbulence and the intermediate state of an overpopulated off-equilibrium system. The generation and clustering of vortices and the annihilation of vortex–antivortex pairs are closely related to the scaling law of a non-thermal fixed point [20–26].

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2. Vortices within GPE

The Bose–Einstein condensate (BEC) in cold atom systems at zero temperature can be well described by the Gross–Pitaevskii (GP) theory as the mean-field approximation of quantum field theories [1]. In GP theory, the ground state and weakly excited states of the condensate are described by the complex wave function \( \psi(r, t) \), which satisfies GPE,

\[
\frac{i\hbar}{\partial t} \psi(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(r, t) + \lambda |\psi(r, t)|^2 \psi(r, t),
\]

where \( \hbar \) is the reduced Planck constant, \( m \) is the particle mass, and the coupling constant \( \lambda \) can reproduce the s-wave scattering length, \( \lambda = 4\pi a_n \hbar^2/m \) in the Born approximation. The investigation on the exact and numerical solutions to GPE improves our understanding on the nonlinear dynamics of matter waves in BEC [30]. In this work, we will focus on the static and rotationally symmetric solution to GPE, the quantum vortex, a kind of topological excitation in a superfluid in presence of the local orbital angular momentum. The wave function can be written in the following form

\[
\psi(r, t) = \sqrt{n_0} \left( \eta = \frac{|\eta|}{\xi} \right) ^{1/2} e^{-i\omega t} ,
\]

where \( n_0 \) is the bulk number density, \( \xi = 1/\sqrt{2m\lambda n_0} \) is the healing length, \( \varphi \) is the azimuthal angle, \( \mu \) is the chemical potential, \( s \) is the winding number which must be an integer to keep the wave function single-valued. The normalized amplitude function \( f(\eta) \) satisfies the nonlinear ordinary differential equation (ODE)

\[
\frac{1}{\eta} \frac{df(\eta)}{d\eta} + \left( \frac{\mu}{\lambda n_0} - \frac{s^2}{\eta^2} \right) f(\eta) - f(\eta)^3 = 0.
\]

Physically, the area modified by a vortex is rather limited, the density profile should return to the bulk value in a region far away from the vortex core, which requires \( \mu/\lambda n_0 = 1 \). So the ODE can be put into the form

\[
f''(\eta) + \frac{1}{\eta} f'(\eta) + \left( 1 - \frac{s^2}{\eta^2} \right) f(\eta) - f(\eta)^3 = 0,
\]

with the boundary conditions \( f(\eta \to 0) = k_s \eta^s \) and \( f(\eta \to \infty) = 1 \). Here \( k_s \) is the connecting parameter, which plays an important role in the vortex solution.

The purpose of this work is to solve equation (4). Without the cubic term, the ODE becomes Bessel’s differential equation with Bessel functions as the formal solution, but the boundary condition at infinity cannot be satisfied. With the cubic term, however, the equation is a nonlinear ODE. It is very hard, if not impossible, to obtain the exact analytical solution to it. So far, we can only find a similar example with an exact solution. It can be easily checked that \( f = \tan (\eta \sqrt{2})/2 \) is one solution to the nonlinear ODE, \( f'' + f(1 - f^2) = 0 \) with the same boundary conditions. This solution is a direct extension of the Riccati equation. In appendix A, we will demonstrate another way to obtain this exact solution which may provide some hints for solving equation (4). The example gives us a little hope that a sufficiently precise numerical solution can guide the guesswork about the possible form of the analytical solution.

For the numerical solution, the differential equation with two-point boundary conditions can be solved with shooting method, which requires a fine tuning of \( k_s \) to achieve the right limit \( f(\eta \to \eta_c) \to 1 \) and \( f'(\eta \to \eta_c) \to 0 \) in the range \( \eta < \eta_c \). The shooting results of \( f(\eta) \) for the winding numbers \( s = 1, 2, 3 \) are shown in figure 1. It seems that shooting works well, but the results are not stable for a large \( \eta_c \), because a rigorous precision in \( k_s \) and an inaccessible small step size in the finite difference are required. Fortunately, we find a relaxation method which can achieve a very high precision in
the whole region of $0 < \eta < \infty$. The technical details will be discussed in the next section.

### 3. Relaxation iteration for a high precision numerical solution

A high precision numerical solution to equation (4) can be achieved by a relaxation iteration. The method is built up with three steps. Firstly, we take a replacement for the target function, $f(\eta) \to \eta^{1/2}(\eta^2 + 1) + h(\eta)$. The auxiliary function $\eta^{1/2}(\eta^2 + 1)$ is to make the unknown function $h(\eta)$ satisfy the boundary condition $h(0) = h(\infty) = 0$, which is convenient for solving the ODE. The function $h(\eta)$ satisfies the nonlinear ODE as follows

$$
d \eta^2 + \frac{1}{\eta} \frac{dh}{d\eta} + \left[ 1 - \frac{\eta^2}{\eta^2} - \frac{3\eta^2}{(1 + \eta^2)^2} \right] h = \eta^3 + \frac{3\eta^3}{1 + \eta^2} + \frac{\eta^3}{\eta^2}(3\eta^2 + \eta^2(2\eta^2 + 1),$$

where we have put all linear terms of $h(x)$ to the left-hand-side. Secondly, we replace the variable $x = \eta/(R + \eta)$, so that the limit $\eta \to \infty$ is shifted to $x \to 1$. The positive number $R$ sets a finite scale, we choose $R = 1$ without loss of generality. The nontrivial change is

$$
\frac{d^2h}{d\eta^2} + \frac{1}{\eta} \frac{dh}{d\eta} + \frac{(1 - x^2)}{R^2} \frac{d^2h}{dx^2} = \frac{2(1 - x^2)}{R^2} \frac{dh}{dx} + \frac{(1 - x^2)^3}{R^2 x} \frac{dh}{dx}. $$

In this way, the ODE is ready for the discretization and iteration. Finally we discretize $x$ as $x_i = i\Delta x$, where $i = 0, \ldots, N$ and the step size is $\Delta x = 1/N$. So the derivatives become

$$
\frac{d^2h}{dx^2} = \frac{h_{i+1} + h_{i-1} - 2h_i}{\Delta x^2},
$$

$$
\frac{dh}{dx} = \frac{h_{i+1} - h_{i-1}}{2\Delta x}.
$$

Then the nonlinear ODE is changed to a set of linear algebraic equation

$$
a_i h_{i+1} + b_i h_i + c_i h_{i-1} = w_i(h_i),$$

for $i = 1, \ldots, N - 1$, where $a_i$, $b_i$, $c_i$, $w_i(h_i)$ are well defined at each point. Because of the well-designed boundary condition, $h_0 = h_N = 0$ does not interfere with the iteration, then equation (8) can be rewritten as

$$
\begin{pmatrix}
    b_1 & c_1 & 0 & \cdots & 0 & 0 & 0 & 1 \\
    a_2 & b_2 & c_2 & \cdots & 0 & 0 & 0 & 0 \\
    0 & a_3 & b_3 & \cdots & 0 & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
    0 & 0 & 0 & \cdots & b_{N-2} & c_{N-2} & 0 & h_{N-3} \\
    0 & 0 & 0 & \cdots & a_{N-2} & b_{N-2} & c_{N-2} & h_{N-3} \\
    0 & 0 & 0 & \cdots & 0 & a_{N-1} & b_{N-1} & h_{N-1} \\
\end{pmatrix}
\begin{pmatrix}
    w_1 \\
    w_2 \\
    w_3 \\
    \vdots \\
    w_{N-3} \\
    w_{N-2} \\
    w_{N-1}
\end{pmatrix} =
\begin{pmatrix}
    h_1 \\
    h_2 \\
    h_3 \\
    \vdots \\
    h_{N-3} \\
    h_{N-2} \\
    h_{N-1}
\end{pmatrix}. $$

We may start by choosing a set of reasonable values for $h_i$ and obtain $w_i(h_i)$, then a new set of $h_i$ can be determined by solving the tridiagonal algebraic equation (9). In this way, a high precision solution can be achieved within dozens of iterations. In the last iteration, the maximum error to $h_i$ is smaller than $10^{-25}$, which means that the algorithm has a fast speed of convergence. The main source to the error comes from the discretization, which can be improved by increasing the number of points $N$. We find the maximum difference between the results with $N = 2^{25}$ and $N = 2^{26}$ is of the order $10^{-16}$, which sets the precision of our numerical solution. The main challenge to go beyond larger $N$ is to handle a larger dimension vector with high precision on a personal computer, that is the reason we stopped at $N = 2^{26}$. For the vector with such a dimension, the iteration to achieve the required precision can be done in a few hours.

For applications, the numerical solution in the form of data sample is not convenient. It is better to look for an approximate analytical solution. The present numerical solution can be used to verify the accuracy of the approximate analytical solution.

The most important input for the approximate analytical solution is the value of connecting parameter $k_i$. We can get it from the numerical solution in the following way. To determine $k_i = \lim_{\eta \to 0} f(\eta)/\eta^2$ with a higher precision, the behavior of $f(\eta)$ near $\eta = 0$ can be parameterized by

$$
f(\eta) \to \left( \frac{\eta}{\eta^2 + \eta^2} \right) \text{tanh}^{-1}(\eta),$$

for example, for winding number $s = 1$, we find that $f(\eta)/\eta$ can be best fitted by $R_8(1 - \eta^2/8)$ for small $\eta$, where $R_8$ is the fitting parameter corresponding to the solution with $N$ grid points. The left panel in figure 2 shows the numerical result for $f(\eta)/\eta - R_8$ with $N = 2^{26}$. The dependence of $R_8$ on $N$ is in table 1 and visualized in the right panel of figure 2.
We may extract the value $k_1 = \lim_{N \to \infty} R_N$ by an extrapolation because these points can be best fitted in the form $R_N - k_1^{\text{ext}} = \beta \gamma^{\log_2 N}$ with fitting parameters $k_1^{\text{ext}}, \beta$ and $\gamma$. Then $k_1^{\text{ext}}$ can be regarded as a high-precision approximation to the exact value of $k_1$. Its reliability will be discussed in the following sections.

In the same way, the extrapolated values of $k_s$ for $s = 2, 3$ can be obtained

$$k_2^{\text{ext}} = 0.153 099 102 859 539,$$
$$k_3^{\text{ext}} = 0.026 183 420 721 62.$$  \hfill (11, 12)

The precision of the connecting parameters is reduced for larger $s$, because it is harder to extract the small $\eta$ behavior of $f(\eta) \propto \eta^2$. But in any way, the present results are precise enough for our purpose. We note that these connecting parameters can be calculated in a semi-analytical scheme [37]. A similar method is discussed in section 5, in which the connecting parameters are traced by choosing the proper root of a polynomial with increasing order. The biggest problem of such semi-analytical schemes is to find the right root of a high-order polynomial, which is computationally expensive, meanwhile the improvement on the precision of $k_s$ is very limited in comparison with the results from the extrapolation method.

4. Two-point Padé approximants for the vortex solution

Analytically, we may try to mimic the solution to equation (4) in terms of Taylor expansion series from both points $\eta = 0$ and $\eta = \infty$ simultaneously. This is the basic idea of two-point Padé approximants. Without loss of generality, we may define $g(\eta)$ by taking a shift $1/2$ in $f(\eta)$, $g(\eta) = f(\eta) - 1/2$, and then expand $g(\eta)$ at $\eta = 0$ and $\eta = \infty$ in the form

$$g(\eta) = \frac{c_0}{2} + \sum_{l=1}^{\infty} c_l \eta^l, \quad \eta \to 0,$$
$$g(\eta) = -\frac{c_0}{2} - \sum_{l=1}^{\infty} c_{-l} \eta^{-l}, \quad \eta \to \infty,$$  \hfill (13, 14)

where $c_0 = -1$ and other coefficients $c_{-l}, \ldots, c_l$ can be derived from equation (4). For $\eta = 0$, by inserting equation (13) into equation (4), we find $c_l = 0$ for $0 < l < s$ and a recursive relation for $c_l$ for $l \geq s$.

Table 1. The numerical values of $R_N$ and $k_1^{\text{ext}}$ extrapolated from $R_N$.

$$\begin{array}{cc}
N = 2^n & R_N \\
\hline
n = 18 & 0.583 189 495 872 \\
n = 19 & 0.583 189 495 8634 \\
n = 20 & 0.583 189 495 8611 \\
n = 21 & 0.583 189 495 860 52 \\
n = 22 & 0.583 189 495 860 37 \\
n = 23 & 0.583 189 495 860 341 \\
n = 24 & 0.583 189 495 860 332 \\
n = 25 & 0.583 189 495 860 3300 \\
n = 26 & 0.583 189 495 860 329 47 \\
\end{array}$$

$$k_1^{\text{ext}} = 0.583 189 495 860 329 28$$

The last term on the left-hand-side of equation (15) comes from the nonlinearity of equation (4). Without this term, the coefficients are just those of Bessel’s functions of the first kind. For the complete form, we can read out that only the coefficients with even/odd indices can be nonzero for the even/odd $s$, and their values are solely determined by the first nonzero one, which is $c_s = k_s$. Take $s = 1$ as an example, we have

$$c_{l+2} = \left[ (l + 2)^2 - s^2 \right] + c_l - \sum_{k_1+k_2+k_3=s} k_1 k_2 k_3 c_{k_1} c_{k_2} c_{k_3} = 0, \quad \text{for } l \geq s.$$  \hfill (15)

For $\eta = \infty$, we insert equation (14) into (4) and obtain $c_{-1} = 0$ and a recursive relation for $c_{-l}$ with $l \geq 2$,

$$c_{-l+2} \left[ (l + 2)^2 - s^2 \right] + c_{-l} = \sum_{k_1+k_2+k_3=s} k_1 k_2 k_3 c_{-k_1} c_{-k_2} c_{-k_3} = 0, \quad \text{for } l \geq 2.$$  \hfill (17)

It can be read out that all coefficients with odd indices are vanishing, the values of coefficients with even indices are solely determined by $s$. For the case $s = 1$, we have...
The coefficients \( c_l \) for \( s = 1 \). The absolute values of \( c_l \) are shown in a logarithmic scale, the sign of \( c_l \) is indicated by the color of the point: red/blue stands for the positive/negative value. The green solid line stands for 1.92 × 2\(^{-24}\) [−1−1/2]. The black solid line stands for 1.125 × 2.512 × 10\(^{34} \). \(^{18}\)

\[
c_{-2} = \frac{1}{2}, \quad c_{-4} = \frac{9}{8}, \quad c_{-6} = \frac{161}{16}, \quad c_{-8} = \frac{24661}{128}.
\]

In Figure 3, we show the values of coefficients \( c_l \) for \( s = 1 \), where \( c_1 \) takes the value of \( k_{ext} \). The absolute values of nonzero coefficients are shown in a logarithmic scale, the sign of each coefficient is indicated by the color of the point: red/blue stands for the positive/negative value. The magnitude of nonzero \( c_l \) with \( l \leq 0 \) is fitted by 1.92 × 2\(^{-24}\) [−1−1/2] as the green solid line. The absolute values of nonzero \( c_l \) with \( l > 0 \) is fitted by 1.125 × 2.512 × 10\(^{34} \) as the black solid line. So that we can read out the convergence radius for the series in equation (13) is about 2.5, while the convergence radius for equation (14) is zero if we take 1/\( \eta \) as the expansion variable. It seems that polynomials of Taylor expansion cannot approximate the solution to equation (4). We have to seek a new type of function to incorporate the boundary conditions from both sides and describe the numerical solution in the whole range \( 0 < \eta < +\infty \).

The two-point Padé approximants in terms of rational functions have the form

\[
\hat{g}_{ij}(\eta) = \frac{P_{ij}(\eta)}{Q_{ij}(\eta)} = \frac{\sum_{l=0}^{m} a_{l} \eta^l}{\sum_{l=0}^{n} b_{l} \eta^l}, \quad \text{with} \quad m = \frac{1}{2} (i + j).
\]

In this form, \( P_{ij}(\eta) \) and \( Q_{ij}(\eta) \) are polynomials with the truncation order \( m \), and \( a_{l} \) and \( b_{l} \) are the coefficients determined by requiring that the expansion of \( \hat{g}_{ij}(\eta) \) at \( \eta \to 0^{+} \) and \( 1/\eta \to 0^{+} \) agrees with equations (13) and (14) up to and with \( c_l \) in equations (13, 14), the polynomials in the numerator and denominator in equation (19) can be constructed in a determinant representation [36],

\[
Q_{ij}(\eta) = \begin{bmatrix}
1 & \eta & \ldots & \eta^{m} \\
c_{i-1} & c_{i-2} & \ldots & c_{i-m-1} \\
& c_{i-2} & \ldots & c_{i-m-2} \\
\vdots & \ddots & \ddots & \vdots \\
& & & c_{i-m} \end{bmatrix},
\]

and \( P_{ij}(\eta) \) is obtained from \( Q_{ij}(\eta) \) by replacing the first row with the vector

\[
\{ S_{m-1}(\eta), \eta S_{m-2}(\eta), \ldots, \eta^{m-1} S_{0}(\eta), \eta^{m} T_{0}(\eta) \}
\]

for \( i \geq m \),

\[
\{ T_{0}(\eta), \eta T_{1}(\eta), \ldots, \eta^{m-1} T_{m-1}(\eta), \eta^{m} T_{m}(\eta) \}
\]

for \( i \leq m \),

where \( S_{l}(\eta) \) and \( T_{l}(\eta) \) are defined as

\[
S_{l}(\eta) = \frac{c_{0}}{2} + \sum_{i=1}^{k} c_{i} \eta^{i},
\]

\[
T_{l}(\eta) = \frac{c_{0}}{2} - \sum_{i=1}^{k} c_{i} \eta^{-i}.
\]

Note that equations (24) and (25) are just the series of equations (13) and (14) up to \( k \) respectively.

In such a way, the two-point Padé approximants for the solution to the ODE (4) can be easily constructed. The truncation index \((i, j)\) sets the size and structure of \( P_{ij} \) and \( Q_{ij} \), while the numerical value of each matrix element can be determined by the recursive relations in equations (15) and (17) with the connecting parameter \( c_{s} = k_{s} \). But in practice, the expected precision in comparison with the numerical solution is not guaranteed by the constructed function (19), although \( k_{s} \) can be determined with extraordinary precision.

The quality of the result depends on the choice of \((i, j)\), so we have to check whether the required accuracy can be achieved for particular values of \( i \) and \( j \). We regard the high precision numerical solution discussed in the previous section as an ‘exact’ solution, from which the accuracy of the approximants can be estimated. For the primary vortex with \( s = 1 \), an economic approximate function is given by setting \( i = 9 \) and \( j = 3 \), which is the best choice for \( m = (i + j)/2 \leq 6 \). The constructed function is parametrized with 12 coefficients in the form

\[
\hat{f}(\eta) = \frac{0.000536403 \, \eta^{6} + 0.00499313 \, \eta^{5} + 0.0279403 \, \eta^{4} + 0.109179 \, \eta^{3} + 0.297503 \, \eta^{2} + 0.583189 \, \eta}{0.000536403 \, \eta^{6} + 0.00499313 \, \eta^{5} + 0.0282085 \, \eta^{4} + 0.111676 \, \eta^{3} + 0.312211 \, \eta^{2} + 0.510131 \, \eta + 1}.
\]

including \( c_{1} \cdot \eta^{-1} \) and \( c_{-1} \eta^{-1} \) respectively. So the residues of the approximants are of the order \( i \) and \( j + 1 \) at the boundaries, i.e.

\[
\hat{g}_{ij}(\eta) - g(\eta) = O(\eta^{i}, \eta^{-j-1}).
\]

The Taylor expansion of this fractional polynomial can reproduce \( c_{1}, \ldots, c_{8} \) for \( \eta \to 0 \) and \( c_{-1}, \ldots, c_{-3} \) for \( 1/\eta \to 0 \). The accuracy of the function with \( i = 9 \) and \( j = 3 \), defined by \( \max(\|f(\eta) - \hat{f}(\eta)\|) \), is about \( 1.2 \times 10^{-3} \), as shown in the left
The accuracy can be significantly improved for larger $m$, as shown in the middle panel of figure 4, the accuracy is about $1.5 \times 10^{-8}$ for the function with $i = 26$ and $j = 10$. The coefficients in this function are listed in appendix B. This approximate function with 56 parameters is good enough for the precise simulation of vortices within GPE.

In the same way, the two-point Padé approximants for the profile functions of vortices with larger winding numbers can be achieved. The coefficients of the fractional polynomials for $s = 2, 3$ are given in appendix B. In both cases, the accuracy is better than $10^{-6}$ in the whole range of $\eta$. It is interesting to see that the approximants with even $s$ contain only even terms in $P_{ij}$ and $Q_{ij}$ because the coefficients $c_i$ with odd $i$ are all vanishing in equations (13) and (14).

Before we work on even higher order functions, we must keep in mind that the coefficients will all change if we choose different $i$ and $j$. The reason is that the polynomials in the numerator or denominator result from matrix determinants, any change to the matrix will give very different polynomials. So we cannot expect the coefficients of polynomials will be determined order by order as in a perturbation theory.

To explore the limit of this method, we try to calculate $P_{ij}(f)$ and $Q_{ij}(f)$ for large $i$ and $j$. The problem is that the matrices of $P_{ij}(f)$ and $Q_{ij}(f)$ involve coefficients $c_i$ that differ dramatically in magnitudes as shown in figure 3, it is a numerical challenge to keep the precision in calculating the determinant of such matrices of large dimension. We found Mathematica can handle these matrices with $i \leq 100$ and $m \leq 60$. The best approximate function that can be accessible corresponds to the matrix for $i = 89$ and $j = 23$, the accuracy is of the order $10^{-14}$, as shown in the right panel of figure 4. The structure and coefficients of the rational functions may indicate some hints for the exact solution to the nonlinear ODE. In appendix A, we give an example of how the Padé approximants help obtain an exact solution to a nonlinear ODE. But for equation (4), we fail to find any hint for an exact solution except approximate functions at very high precision.

5. Error estimation and challenge

The precision of Padé approximants cannot be improved by simply increasing the truncation order. The asymptotic errors for both boundaries can be estimated as

\[ |g(\eta) - \hat{g}_{ij}(\eta)| = \left| \frac{D_{i-m,m}}{D_{i-m-1,m-1}} \right| \eta^j(1 + O(\eta)) \]

for $\eta \to 0$, \hspace{1cm} (27)

\[ |g(\eta) - \hat{g}_{ij}(\eta)| = \left| \frac{D_{i-m-1,m}}{D_{i-m,m-1}} \right| \eta^{-j}(1 + O(\eta^{-1})) \]

for $\eta \to \infty$, \hspace{1cm} (28)

with $D_{r,s}$ being the determinant of the coefficient matrix

\[ D_{r,s} = \begin{vmatrix} c_r & c_{r+1} & \cdots & c_{r+j} \\ c_{r-1} & c_r & \cdots & c_{r+j-1} \\ \vdots & \vdots & \ddots & \vdots \\ c_{r-t} & c_{r-t+1} & \cdots & c_r \end{vmatrix}. \hspace{1cm} (29) \]

The error for small $\eta$ is controlled by the ratio $|D_{i-m,m}/D_{i-m-1,m-1}|$. To have an intuitive idea about the ratio, we estimate it as a function of $m$ for the case $i = j = m$. As shown in the left panel of figure 5, the ratio can be approximated as $10^2 \times 5.5^{-m}$. This feature reveals that the convergence radius of $\hat{g}_{ij}$ has been extended from 2.5 to 5.5 by Padé approximants for small $\eta$. For large $\eta$, the dependence of $|D_{-1,m}/D_{0,m-1}|$ on $m$ is shown in the right panel of figure 5 and can be described by $10^{-10} \times 15^m$. This means that the error is under control for $|\eta| > 18$, or the convergence radius for $1/|\eta|$ is extended from 0 to 1/18. Although the change of the convergence radius is small, the coverage range of the approximants is expanded significantly. Actually, this is a remarkable progress of Padé approximants which aim to reproduce a complicated function from both boundaries simultaneously. Inside the gap between two convergence regions, the rational function connects both regions smoothly, which should reproduce the target function with a similar or slightly worse precision if the target function does not contain a singularity in the gap. The error can be further reduced by fine-tuning of $i$ and $j$ if the target function is known with higher precision. As we have already shown in figure 4, the vortex profile function can be reproduced with high accuracy, and the behaviors of errors can be well understood as discussed above.

In the description of Padé approximants for vortex profiles, we find that $P_{ij}$, $Q_{ij}$ and $D_{i,j}$ are sensitive to the connecting parameter $k_s$. Since the corresponding matrices have a similar structure, we take $D_{i,j}$ as an example to discuss its dependence on $k_s$. For simplicity, we look at $D_{0,m}$ and $k_1$. From equation (29), $D_{0,m}$ can be expressed as a polynomial of $c_j$ and the order increases fast with the dimension of the matrix. We find that $D_{0,m}$ has some real roots, denoted as $c_j'$, which are very close to $k_1$. The distance between each $c_j'$ and
k_1 is shown in figure 6, where the magnitude is plotted in logarithm scale and the sign is marked by color. A bunch of roots near k_1 indicate that D_0,m varies dramatically when c_1 approaches k_1. So it can be understood that a small deviation from k_1 will lead to an uncontrollable variation of D_{ij} when the dimension of the matrix becomes large. Similar behavior is also observed in P_{ij} and Q_{ij} as functions of c_1. So the accuracy of the Padé approximants for large m strongly depends on the precision of k_1. As shown in figure 7, for the best result that we find (the right panel of figure 4), a very small change in the value of k_1 leads to a significant increase in the error of the approximants. So the precision of k_1 is crucial for that of Padé approximants for large m.

The minimal distance in figure 6 can be extremely small for large m, it seems that this feature can be employed to find the asymptotic value of k_1 from c_1 with a carefully chosen initial value and iteration of increasing m. Technically, we can set the only possible root of D_{0,4} as the initial value, and replace it with one root of D_{0,5} which is real and closest to the original one. Repeat this procedure, a chain of the closest root can be found, approaching the true value of k_1. As shown in figure 6, the bottom line is traceable without knowing k_1 at first. This idea is workable for m < 80, with the precision at the level of 10^{-12}. But for even larger m, it is difficult to find the right root of a high-order polynomial, because the density of roots near k_1 increases while the minimal distance between them decreases exponentially, which raises the risk of finding wrong roots. This is the reason why we do not seek the value of k_1 from roots of D_{ij} but import the extrapolated value from a series of numerical solutions with a reliable precision. At the present stage, with Mathematica running on a laptop, we can confirm the value of k_1 with 17 significant digits, which helps us to promote the precision of the two-point Padé approximants to 10^{-14}. The method may help us to search for the exact solution of the vortex profile.

6. Summary and conclusion

Understanding the vortex dynamics is important for the study of superfluids and many other physical systems. Due to the nonlinear nature of the vortex dynamics, the evolution of the vortex can only be studied in a perturbative way, which requires a high precision solution to the stationary wave function of the vortex. The nonlinear ODE for the vortex profile function can be solved numerically with high precision.

For practical applications, we have constructed semi-analytical solutions to this problem with two-point Padé approximants. These solutions are presented with simple rational functions, which have a high accuracy and are ready for use in the precise simulation of the vortex dynamics. The
coefficients of rational functions strongly depend on the value of the connecting parameter which can be obtained in high precision from an extrapolation of the numerical solution or a systematic root-finding in a series of polynomials.

The accuracy of the approximate solutions can be improved significantly with a reasonable extension in the order of rational functions. With a systematic scan of the truncation orders, the best accuracy is found to be at the order of $10^{-15}$. The errors of the approximate functions and the limitation of two-point Padé approximants are discussed, which can extend our understanding on the nonlinearity of the vortex dynamics. This investigation may provide the clue for an exact solution to the vortex profile function.

The methods and algorithms developed in this work for high precision solutions to the vortex equation can be applied to other nonlinear systems, such as the Schrödinger–Poisson problem [38, 39], the shape and properties of Bose stars formed by dark matter through the universal gravitational interaction and so on.

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Appendix A. An example for exact solution with two-point Padé approximants

We consider the nonlinear ODE

$$\frac{d^2 f}{dx^2}(x) + f(x) - f^3(x) = 0, \quad (A1)$$

with the boundary conditions $f(0)=0$ and $f(\infty) = 1$. At the zero point, we may insert the formal solution

$$f(x) = \sum_{n=0}^{\infty} c_n x^n, \quad (A2)$$

into the ODE. It is easy to check that all even terms are vanishing, i.e. $c_{2k} = 0$ for $k = 0, 1, \cdots$. The odd terms satisfy the recurrence relation

$$c_{n+2}(n+2)(n+1) + c_n - \sum_{k_1+k_2+k_3=n} c_{k_1}c_{k_2}c_{k_3} = 0. \quad (A3)$$

The only unsettled parameter is $c_1$, which other coefficients can be expressed, for example, we have the following expressions for $c_3, \cdots, c_9$ in terms of $c_1$

$$\begin{align*}
c_1 &= -\frac{1}{3!} c_0, \\
c_5 &= \frac{1}{5!}(c_1 + 6c_1^3), \\
c_7 &= -\frac{1}{7!} (c_1 + 6c_1^3), \\
c_9 &= \frac{1}{9!} (c_1 + 612c_1^3 + 756c_1^5). \quad (A4)
\end{align*}$$

We may represent the solution in the form of Padé approximants

$$f^{(N)}(x) = \sum_{i=0}^{N} a_i x^i \sum_{j=0}^{N} b_j x^j, \quad (A5)$$

Because the solution is determined by the ratio, it is natural to demand $b_0 = 1$. Because $c_0 = 0$, we can set $a_0 = 0$. Other coefficients should satisfy

$$a_i = \sum_{j=0}^{N} b_j c_{i-j}, \quad \text{for } 1 \leq i \leq N. \quad (A6)$$

For the boundary condition at $x \to \infty$, we can change the variable to $z=1/x$, so that equation (A1) can be rewritten as

$$z^4 \frac{d^2 f}{dz^2}(z) + 2z^3 \frac{df}{dz}(z) + f(z) - f^3(z) = 0. \quad (A7)$$

Then we can take the formal solution in the form

$$f(z) = \sum_{i=0}^{\infty} d_i z^i. \quad (A8)$$

It is easy to obtain $d_0 = 1$ and $d_i = 0$ for $i > 0$. So there is another constraint for coefficients

$$a_i = \sum_{j=0}^{N} b_j d_{i-j} = b_i, \quad \text{for } 1 \leq i \leq N. \quad (A9)$$

Combining equations (A6) and (A9), we obtain a set of linear equations for $(a_1, \cdots, a_N)$ or $(b_1, \cdots, b_N)$. We may write the equations into a matrix form. As an example, the equations for $N = 5$ read

$$\begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
-c_1 & 1 & 0 & 0 & 0 \\
0 & -c_1 & 1 & 0 & 0 \\
\frac{c_1}{6} & 0 & -c_1 & 1 & 0 \\
0 & \frac{c_1}{6} & 0 & -c_1 & 1
\end{pmatrix}
\begin{pmatrix}
b_1 \\
b_2 \\
b_3 \\
b_4 \\
b_5
\end{pmatrix} =
\begin{pmatrix}
c_1 \\
0 \\
-\frac{c_1}{6} \\
0 \\
\frac{c_1}{120}
\end{pmatrix}. \quad (A10)$$

Because the matrix is already in a triangle form, the solution can be easily obtained

$$\begin{pmatrix}
a_1 \\
a_2 \\
a_3 \\
a_4 \\
a_5
\end{pmatrix} =
\begin{pmatrix}
b_1 \\
b_2 \\
b_3 \\
b_4 \\
b_5
\end{pmatrix} =
\begin{pmatrix}
c_1 \\
c_1^2 \\
c_1^3 \frac{1}{6} \\
c_1^4 \frac{1}{3} c_1^2 \\
c_1^5 \frac{9}{20} c_1^3 + \frac{1}{120} c_1^5
\end{pmatrix}. \quad (A11)$$
To determine the value of $c_1$, we may demand one more constraint on the solution by taking $a_{N+1} = b_{N+1} = 0$, which can be written as
\[
\sum_{j=1}^{N} b_j c_{N+1-j} + c_{N+1} = 0.
\] (A12)

It gives an algebra equation for $c_1$. As an example, for $N=5$, the equation reads
\[
\frac{c_1^2}{90} (90c_1^4 - 51c_1^2 + 4) = 0.
\] (A13)

The meaningful root to the above equation is $\sqrt{(51 + 3\sqrt{123})}/180 \approx 0.687481$. In this way, we can get a series of $c_1$ values 0.69976, 0.704416, 0.706143, 0.706768, 0.706989 for $N=6, 7, 8, 9, 10$ respectively. We may check that the approximate value of $c_1$ becomes closer to $\sqrt{2}/2 \approx 0.707107$ for large $N$. If we set $c_1 = \sqrt{2}/2$, we find the solution in equation (A11) can be simplified to $a_i = b_i = (\sqrt{2}y/(2 \cdot i!)$. So the solution can be put into the form
\[
f^{(N)}(x) = \frac{\sum_{i=0}^{N} (\sqrt{2}x)^i/(2 \cdot i!)}{1 + \sum_{i=0}^{N} (\sqrt{2}x)^i/(2 \cdot i!)}
= \frac{\sum_{i=0}^{N} (\sqrt{2}x)^i}{\sum_{i=0}^{N} (\sqrt{2}x)^i + 1}.
\] (A14)

It happens to give $f(x) = \tanh(x/\sqrt{2})$ if we send $N$ to $\infty$.

**Appendix B. Coefficients in approximate functions for vortex profiles**

In this appendix we list the coefficients in approximate functions in (19) with which one can reproduce the vortex profiles in high accuracy.

| $l$ | $\alpha_l$ | $\beta_l$ |
|-----|------------|------------|
| 0   | 0          | 1.000 000 000 |
| 1   | 5.831 894 959 $\times 10^{-1}$ | 5.873 264 261 $\times 10^{-1}$ |
| 2   | 3.425 226 024 $\times 10^{-1}$ | 5.455 940 613 $\times 10^{-1}$ |
| 3   | 2.452 860 386 $\times 10^{-1}$ | 2.468 318 072 $\times 10^{-1}$ |
| 4   | 1.011 343 919 $\times 10^{-1}$ | 1.145 178 304 $\times 10^{-1}$ |
| 5   | 3.831 447 420 $\times 10^{-2}$ | 3.898 275 190 $\times 10^{-2}$ |
| 6   | 1.137 856 193 $\times 10^{-2}$ | 1.179 179 362 $\times 10^{-2}$ |
| 7   | 2.909 882 040 $\times 10^{-3}$ | 2.971 398 890 $\times 10^{-3}$ |
| 8   | 6.323 721 506 $\times 10^{-4}$ | 6.423 893 504 $\times 10^{-4}$ |
| 9   | 1.180 693 171 $\times 10^{-4}$ | 1.194 567 590 $\times 10^{-4}$ |
| 10  | 1.905 344 120 $\times 10^{-5}$ | 1.922 168 115 $\times 10^{-5}$ |
| 11  | 2.672 381 372 $\times 10^{-6}$ | 2.690 240 172 $\times 10^{-6}$ |
| 12  | 3.271 123 471 $\times 10^{-7}$ | 3.287 644 644 $\times 10^{-7}$ |
| 13  | 3.497 660 717 $\times 10^{-8}$ | 3.510 863 602 $\times 10^{-8}$ |
| 14  | 3.524 331 773 $\times 10^{-9}$ | 3.526 312 251 $\times 10^{-9}$ |
| 15  | 2.613 493 838 $\times 10^{-10}$ | 2.618 418 071 $\times 10^{-10}$ |
| 16  | 1.786 780 526 $\times 10^{-11}$ | 1.788 474 199 $\times 10^{-11}$ |
| 17  | 9.848 466 014 $\times 10^{-13}$ | 9.848 466 014 $\times 10^{-13}$ |
| 18  | 3.387 345 177 $\times 10^{-14}$ | 3.387 345 177 $\times 10^{-14}$ |

| $l$ | $\alpha_l$ | $\beta_l$ |
|-----|------------|------------|
| 0   | 0          | 1.000 000 000 |
| 1   | 1.530 991 029 $\times 10^{-1}$ | 1.530 991 029 $\times 10^{-1}$ |
| 2   | 5.458 897 193 $\times 10^{-2}$ | 5.458 897 193 $\times 10^{-2}$ |
| 3   | 5.406 591 644 $\times 10^{-3}$ | 5.406 591 644 $\times 10^{-3}$ |
| 4   | 2.685 749 628 $\times 10^{-4}$ | 2.685 749 628 $\times 10^{-4}$ |
| 5   | 7.837 336 242 $\times 10^{-6}$ | 7.837 336 242 $\times 10^{-6}$ |
| 6   | 1.472 555 945 $\times 10^{-7}$ | 1.472 555 945 $\times 10^{-7}$ |
| 7   | 1.934 727 229 $\times 10^{-9}$ | 1.934 727 229 $\times 10^{-9}$ |
| 8   | 1.693 952 735 $\times 10^{-11}$ | 1.693 952 735 $\times 10^{-11}$ |
| 9   | 1.522 898 667 $\times 10^{-13}$ | 1.522 898 667 $\times 10^{-13}$ |

| $l$ | $\alpha_l$ | $\beta_l$ |
|-----|------------|------------|
| 0   | 0          | 1.000 000 000 |
| 1   | 1.530 991 029 $\times 10^{-1}$ | 1.530 991 029 $\times 10^{-1}$ |
| 2   | 5.458 897 193 $\times 10^{-2}$ | 5.458 897 193 $\times 10^{-2}$ |
| 3   | 5.406 591 644 $\times 10^{-3}$ | 5.406 591 644 $\times 10^{-3}$ |
| 4   | 2.685 749 628 $\times 10^{-4}$ | 2.685 749 628 $\times 10^{-4}$ |
| 5   | 7.837 336 242 $\times 10^{-6}$ | 7.837 336 242 $\times 10^{-6}$ |
| 6   | 1.472 555 945 $\times 10^{-7}$ | 1.472 555 945 $\times 10^{-7}$ |
| 7   | 1.934 727 229 $\times 10^{-9}$ | 1.934 727 229 $\times 10^{-9}$ |
| 8   | 1.693 952 735 $\times 10^{-11}$ | 1.693 952 735 $\times 10^{-11}$ |
| 9   | 1.522 898 667 $\times 10^{-13}$ | 1.522 898 667 $\times 10^{-13}$ |
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