

Thomas–Fermi ground state in a PT -symmetric confining potential

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Introduction

The Gross-Pitaevskii equation with a harmonic confining potential can be written in the semi-classical form

$$i \varepsilon u_t = -\varepsilon^2 u_{xx} + x^2 u - u + |u|^2 u.$$

The limit $\varepsilon \rightarrow 0$ for large-density stationary states is referred to as the **Thomas–Fermi** limit since L.H. Thomas (1927) and E. Fermi (1928).

Theorem (Ignat & Milot, 2006): For sufficiently small $\varepsilon > 0$, there exists a real-valued, positive-definite global minimizer of the Gross–Pitaevskii energy

$$E_\varepsilon(u) = \int_{\mathbb{R}} \left(\varepsilon^2 |u_x|^2 + x^2 |u|^2 - |u|^2 + \frac{1}{2} |u|^4 \right) dx$$

in the energy space

$$X = \{u \in H^1(\mathbb{R}) : xu \in L^2(\mathbb{R})\}.$$

Ground state in the variational theory

Let η_ε be a global minimizer of E_ε . From Euler–Lagrange equations, it solves

$$-\varepsilon^2 \eta_\varepsilon''(x) + (\eta_\varepsilon^2 + x^2 - 1) \eta_\varepsilon(x) = 0, \quad x \in \mathbb{R}.$$

The formal limit for the ground state is

$$\eta_0(x) = \begin{cases} (1 - x^2)^{1/2}, & \text{for } |x| < 1, \\ 0, & \text{for } |x| > 1, \end{cases}$$

By variational analysis via sub- and super-solutions, it was found that

$$\begin{cases} 0 \leq \eta_\varepsilon(x) \leq C \varepsilon^{1/3} \exp\left(\frac{1-x^2}{4\varepsilon^{2/3}}\right) & \text{for } |x| \geq 1, \\ (1 - C\varepsilon^{1/3})(1 - x^2)^{1/2} \leq \eta_\varepsilon(x) \leq (1 - x^2)^{1/2} & \text{for } |x| \leq 1 - \varepsilon^{1/3}, \end{cases}$$

where C is ε -independent.

Ground state in the asymptotic theory

Let

$$\eta_\varepsilon(x) = \varepsilon^{1/3} \nu_\varepsilon(y), \quad y = \frac{1-x^2}{\varepsilon^{2/3}}$$

and rewrite the stationary equation for $\nu_\varepsilon(y)$:

$$4(1 - \varepsilon^{2/3} y) \nu_\varepsilon''(y) - 2\varepsilon^{2/3} \nu_\varepsilon'(y) + y \nu_\varepsilon(y) - \nu_\varepsilon^3(y) = 0, \quad y \in (-\infty, \varepsilon^{-2/3}).$$

The formal limit $\varepsilon \rightarrow 0$ gives the Painlevé–II equation

$$4\nu''(y) + y\nu(y) - \nu^3(y) = 0, \quad y \in \mathbb{R},$$

that admits a unique [Hastings–McLeod \(1986\)](#) solution $\nu_0(y)$ satisfying

$$\nu_0(y) \sim y^{1/2} \quad \text{as } y \rightarrow +\infty, \quad \nu_0(y) \sim |y|^{-1/4} e^{-|y|^{3/2}/3} \quad \text{as } y \rightarrow -\infty.$$

[Boscolo et al. \(2002\)](#); [Konotop & Kevrekidis \(2003\)](#); [Aftalion et al. \(2003\)](#)

Rigorous result

Theorem (C. Gallo & D.P., 2011): Let ν_0 be the unique Hastings–McLeod solution of the Painlevé II equation. Then, there exists $\varepsilon_0 > 0$ and $C_0 > 0$ s.t. for every $\varepsilon \in (0, \varepsilon_0)$, there is

$$R_\varepsilon \in L^\infty(-\infty, \varepsilon^{-2/3}), \quad \text{with} \quad \|R_\varepsilon\|_{L^\infty} \leq C_0, \quad \lim_{y \rightarrow -\infty} R_\varepsilon(y) = 0,$$

such that for every $x \in \mathbb{R}$,

$$\eta_\varepsilon(x) = \varepsilon^{1/3} \nu_0 \left(\frac{1 - x^2}{\varepsilon^{2/3}} \right) + \varepsilon R_\varepsilon \left(\frac{1 - x^2}{\varepsilon^{2/3}} \right).$$

- The proof is based on the fixed-point arguments.
- The method works for radially symmetric states in dimensions 2 and 3.
- More complicated cases: non-radial potentials (Karali & Sourdis, 2013); coupled Gross–Pitaevskii equations (Gallo, 2014).

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PT-symmetric potentials

The stationary Gross-Pitaevskii equation with a harmonic confining and PT-symmetric potentials takes the form

$$\mu U(X) = (-\partial_X^2 + X^2 + 2i\alpha W(X) + |U(X)|^2) U(X), \quad X \in \mathbb{R},$$

where $\mu \in \mathbb{R}$ is the chemical potential, W is real and odd, and $\alpha \in \mathbb{R}$: $i\alpha W(-X) = -i\alpha W(X)$.

In what follows, we take $W(X) = X$. The spectrum of

$$L_0 := -\partial_X^2 + X^2 + 2i\alpha X = -\partial_X^2 + (X + i\alpha)^2 + \alpha^2$$

is purely discrete and real. The ground state bifurcates from the smallest eigenvalue $\mu_0 = 1 + \alpha^2$ and exists for $\mu \geq \mu_0$ (Zezyulin & Konotop, 2012).

The Thomas–Fermi limit corresponds to $\mu \rightarrow \infty$ and rescaling $\mu = \varepsilon^{-1}$, $U(X) = \varepsilon^{-1/2} u(x)$, and $x = \varepsilon^{1/2} X$:

$$\varepsilon^2 u''(x) + \left(1 - x^2 - 2i\alpha \varepsilon^{1/2} x - |u(x)|^2\right) u(x) = 0, \quad x \in \mathbb{R}.$$

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Numerical approximations

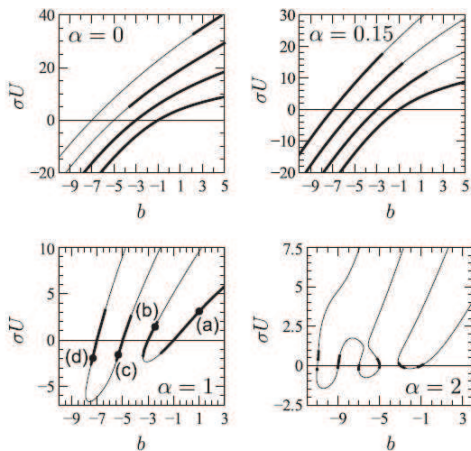


Figure : Numerical approximations: D.Zezyulin–V. Konotop, PRA **85** (2012), 043840.

PT-symmetric ground state

We are looking for the ground state with $|u(x)| > 0$ for all $x \in \mathbb{R}$. The ground state is *PT*-symmetric if $u(-x) = \bar{u}(x)$, when we can write

$$u(x) = \varphi(x) e^{\epsilon^{-1} \int_{-\infty}^x \xi(x') dx'}$$

and obtain

$$\begin{cases} (1 - x^2 - \varphi^2(x) - \xi^2(x)) \varphi(x) = -\epsilon^2 \varphi''(x), \\ (\varphi^2 \xi)'(x) = 2\eta x \varphi^2(x), \end{cases} \quad x \in \mathbb{R},$$

where $\alpha = \epsilon^{1/2} \eta$. Both φ and ξ are real and even.

Under the condition $\lim_{x \rightarrow \pm\infty} \varphi^2(x) \xi(x) = 0$, one can uniquely write

$$\xi(x) = \frac{2\eta}{\varphi^2(x)} \int_{-\infty}^x s \varphi^2(s) ds,$$

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Limiting Thomas–Fermi state

Formal limit $\epsilon = 0$ corresponds to the compact approximation

$$\begin{cases} 1 - x^2 - \varphi^2(x) - \xi^2(x) = 0, \\ (\varphi^2 \xi)'(x) = 2\eta x \varphi^2(x), \end{cases} \quad x \in [-1, 1],$$

subject to the boundary conditions $\varphi(\pm 1) = \xi(\pm 1) = 0$. Again, we can write

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Theorem (C. Gallo & D.P., 2014): There exists $\eta_0 > 0$ s.t. for any $|\eta| < \eta_0$, there exists a unique solution $\varphi_{\text{TF}} \in C^\infty(-1, 1)$ s.t. $\varphi_{\text{TF}}(x) > 0$ for all $x \in (-1, 1)$ and

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Numerical approximations of the limiting state

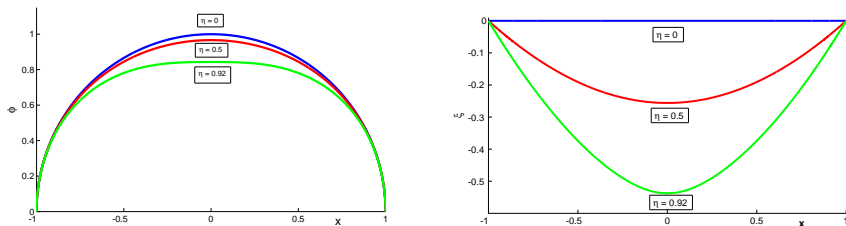


Figure : Components φ (left) and ξ (right) for the numerical solution to the limiting problem for three different values of η .

Justification of the limiting Thomas–Fermi state

Setting

$$\varphi(x) = \varepsilon^{1/3} \nu(y), \quad \xi(x) = \varepsilon^{2/3} \chi(y), \quad y = \frac{1-x^2}{\varepsilon^{2/3}}.$$

we obtain for $y \in (-\infty, \varepsilon^{-2/3})$,

$$\begin{cases} 4\nu''(y) + y\nu(y) - \nu^3(y) = \varepsilon^{2/3} (4y\nu''(y) + 2\nu'(y) + \chi^2(y)\nu(y)), \\ (\nu^2\chi)'(y) = -\eta\nu^2(y), \end{cases}$$

subject to the decay condition $\nu(y) \rightarrow 0$ as $y \rightarrow -\infty$.

Recall the unique Hastings–McLeod solution ν_0 of the Painlevé–II equation

$$4\nu''(y) + y\nu(y) - \nu^3(y) = 0, \quad y \in \mathbb{R},$$

satisfying

$$\nu_0(y) \sim y^{1/2} \quad \text{as } y \rightarrow +\infty \quad \text{and} \quad \nu_0(y) \sim |y|^{-1/4} e^{-|y|^{3/2}/3} \quad \text{as } y \rightarrow -\infty.$$

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Persistence of the Hastings–McLeod solution

Conjecture (C. Gallo & D.P., 2014): Let ν_0 be the Hastings–McLeod solution of the Painlevé-II equation. For any $q > \frac{5}{6}$, there exist $\varepsilon_q > 0$, $\eta_q > 0$, and $C_q > 0$ s.t. for every $\varepsilon \in (0, \varepsilon_q)$ and $|\eta| < \eta_q \varepsilon^q$, there exists a unique solution $\nu_P, \chi_P \in C^\infty(-\infty, \varepsilon^{-2/3})$ s.t. $\nu_P(y) > 0$ for all $y \in (-\infty, \varepsilon^{-2/3})$ and

$$\sup_{y \in (-\infty, \varepsilon^{-2/3})} |\nu_P(y) - \nu_0(y)| \leq C_q \begin{cases} \varepsilon^{2q-4/3} |\log(\varepsilon)|^{1/2}, & q \leq 1, \\ \varepsilon^{2/3}, & q > 1. \end{cases}$$

- An alternating fixed-point iteration scheme is proposed but the convergence of the scheme is only confirmed numerically.
- Since η is ε -dependent and small, for every $x \in (-1, 1)$, we have

$$\varepsilon^{2/3} \nu_P^2(y) \rightarrow 1 - x^2 \quad \text{as } \varepsilon \rightarrow 0.$$

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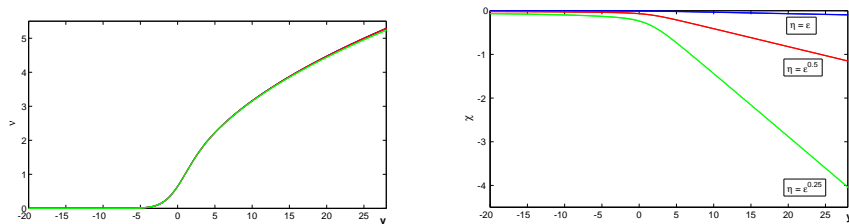


Figure : Components ν (left) and χ (right) for the numerical solution to the coupled system with $\epsilon = 0.0067$ and three different values of η .

Proof of Theorem on the limiting Thomas–Fermi state

We are solving

$$\begin{cases} 1 - x^2 - \varphi^2(x) - \xi^2(x) = 0, \\ (\varphi^2\xi)'(x) = 2\eta x\varphi^2(x), \end{cases} \quad x \in [-1, 1],$$

subject to the boundary conditions $\varphi(\pm 1) = \xi(\pm 1) = 0$.

Let $z := 1 - x^2$ and $\omega(z) := \varphi^2(x) = z - \xi^2(z)$. Then, we are solving the first-order differential equation

$$\frac{d}{dz} (z\xi - \xi^3) = -\eta(z - \xi^2), \quad z \in [0, 1].$$

subject to the boundary condition $\xi(0) = 0$. In fact, we have

$$\xi(z) = -\frac{1}{2}\eta z \left[1 + \frac{1}{8}\eta^2 z + \mathcal{O}(\eta^4 z^2) \right].$$

Unfolding the singularities

Writing $\xi(z) = -\frac{1}{2}\eta z\psi(\zeta)$ and $\zeta := \eta^2 z$, we obtain

$$\frac{d\psi}{d\zeta} = \frac{4(1-\psi) - \zeta\psi^2(1 - \frac{3}{2}\psi)}{2\zeta(1 - \frac{3}{4}\zeta\psi^2)}, \quad \zeta \in [0, \eta^2],$$

subject to $\psi(0) = 1$.

Let $\tau := \log(\zeta)$ for $\zeta > 0$. Then, the first-order equation becomes a planar autonomous dynamical system

$$\dot{\zeta} = \zeta, \quad \dot{\psi} = \frac{4(1-\psi) - \zeta\psi^2(1 - \frac{3}{2}\psi)}{2(1 - \frac{3}{4}\zeta\psi^2)}$$

where $(\zeta, \psi) = (0, 1)$ is an equilibrium point. It is a saddle point with an unstable manifold of the linearized system along the line $\psi - 1 = \frac{1}{8}\zeta$.

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The Thomas–Fermi limiting state

By the Unstable Manifold Theorem, there exists a unique trajectory in the right half-plane (ζ, ψ) such that $\psi \rightarrow 1$ as $\zeta \rightarrow 0$. The solution exists locally for $\tau \in (-\infty, \tau_0)$ for some $\tau_0 \in \mathbb{R}$ or for $\zeta \in [0, \zeta_0)$ for some η -independent $\zeta_0 > 0$.

Unfolding back the previous transformations, the solution exists for $z \in [0, \zeta_0 \eta^{-2})$, which includes $[0, 1]$ if η is sufficiently small. Then, $\varphi_{\text{TF}}(x) = \sqrt{1 - x^2 - \xi^2(1 - x^2)}$ is the Thomas–Fermi limiting state.

Theorem (C. Gallo & D.P., 2014): There exists $\eta_0 > 0$ s.t. for any $|\eta| < \eta_0$, there exists a unique solution $\varphi_{\text{TF}} \in C^\infty(-1, 1)$ s.t.

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Remark: The solution breaks at $\eta = \eta_0$, when $\xi'(x)$ becomes infinite at $x = 0$.

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Towards the proof of Conjecture

We are solving for $y \in (-\infty, \varepsilon^{-2/3})$

$$\begin{cases} 4\nu''(y) + y\nu(y) - \nu^3(y) = \varepsilon^{2/3} (4y\nu''(y) + 2\nu'(y) + \chi^2(y)\nu(y)), \\ (\nu^2\chi)'(y) = -\eta\nu^2(y), \end{cases}$$

subject to the decay condition $\nu(y) \rightarrow 0$ as $y \rightarrow -\infty$.

- 1 Assume that $\chi \in L^\infty(-\infty, \varepsilon^{-2/3})$ is given with a suitable behavior in ε and η . Prove that there exists a solution of the first equation for $\nu \in L^2(-\infty, \varepsilon^{-2/3}) \cap C^0(-\infty, \varepsilon^{-2/3})$ near the Hastings–McLeod solution.
- 2 Assume that $\nu \in L^2(-\infty, \varepsilon^{-2/3}) \cap C^0(-\infty, \varepsilon^{-2/3})$ is given with a suitable behavior in ε and η . Prove that there exists a solution of the second equation for $\chi \in L^\infty(-\infty, \varepsilon^{-2/3})$.
- 3 Develop an alternating iterative scheme and show that it converges to a suitable solution of the coupled system.

Step 1: mapping $\chi \rightarrow \nu$

Theorem

Let ν_0 be the Hastings–McLeod solution of the Painlevé-II equation. Let $\chi \in L^\infty(-\infty, \varepsilon^{-2/3})$ satisfy for some (ε, η) -independent $C_+ > 1$ and $C_- > 0$:

$$\begin{aligned} C_+^{-1} |\eta| y &\leq |\chi(y)| \leq C_+ |\eta| (1 + y), & y \in (0, \varepsilon^{-2/3}) \\ |\chi(y)| &\leq C_- |\eta|, & y \in (-\infty, 0). \end{aligned}$$

For any $q > \frac{5}{6}$, there exist $\varepsilon_q > 0$, $\eta_q > 0$, and $C_q > 0$ s.t. for every $\varepsilon \in (0, \varepsilon_q)$ and $|\eta| < \eta_q \varepsilon^q$, there exists a unique solution $R \in L^2 \cap C^0(-\infty, \varepsilon^{-2/3})$ s.t. $\nu(y) = \nu_0(y) + R(y) > 0$ for all $y \in (-\infty, \varepsilon^{-2/3})$ and

$$\|R\|_{L^\infty(-\infty, \varepsilon^{-2/3})} \leq C_q \begin{cases} \varepsilon^{2q-4/3} |\log(\varepsilon)|^{1/2}, & \text{if } q \leq 1, \\ \varepsilon^{2/3}, & \text{if } q > 1. \end{cases}$$

Furthermore, if $\nu_{1,2}$ correspond to $\chi_{1,2}$, then there exists an ε -independent positive constant C such that

$$\|\nu_1 - \nu_2\|_{L^2 \cap L^\infty} \leq C \varepsilon^{2/3} \|\chi_1^2 - \chi_2^2\|_{L^\infty} \|\nu_1\|_{L^2}.$$

Decay of the solution $\nu(y)$ as $y \rightarrow -\infty$

Recall the growth and decay of the Hastings–McLeod solution ν_0 :

$$\nu_0(y) \sim y^{1/2} \quad \text{as } y \rightarrow +\infty \quad \text{and} \quad \nu_0(y) \sim |y|^{-1/4} e^{-|y|^{3/2}/3} \quad \text{as } y \rightarrow -\infty.$$

Because R is bounded, $\nu(y) = \nu_0(y) + R(y)$ has the same growth at $y = \mathcal{O}(\varepsilon^{-2/3})$ as $\varepsilon \rightarrow 0$. On the other hand, the WKB theory for

$$\varepsilon^2 \varphi''(x) + (1 - x^2 - \xi_\infty^2) \varphi(x) = 0,$$

with $\xi_\infty := \lim_{|x| \rightarrow \infty} \xi(x)$, shows that there is $\gamma > 0$ such that

$$\nu(y) \underset{y \rightarrow -\infty}{\sim} \gamma |y|^{\frac{1-\varepsilon - \xi_\infty^2}{4\varepsilon}} e^{-\frac{|y|}{2\varepsilon^{1/3}}}.$$

Therefore, $\nu(y)$ decays much slower than $\nu_0(y)$ as $y \rightarrow -\infty$.

Step 2: mapping $\nu \rightarrow \chi$

We integrate the second equation of the system

$$(\nu^2 \chi)'(y) = -\eta \nu^2(y) \quad \Rightarrow \quad \chi(y) = -\frac{\eta}{\nu^2(y)} \int_{-\infty}^y \nu^2(s) ds.$$

Lemma

Let $\nu \in L^2 \cap C^0(-\infty, \varepsilon^{-2/3})$ satisfy for (ε, η) -independent $C_+ > 1$ and $C_- > 0$:

$$\begin{aligned} C_+^{-1} y \leq \nu^2(y) \leq C_+(1+y), \quad y \in (0, \varepsilon^{-2/3}), \\ \frac{1}{\nu^2(y)} \int_{-\infty}^y \nu^2(s) ds \leq C_-, \quad y \in (-\infty, 0). \end{aligned}$$

Then, $\chi \in L^\infty(-\infty, \varepsilon^{-2/3})$ is well-defined and satisfies

$$\begin{aligned} C_+^{-1} |\eta| y \leq |\chi(y)| \leq C_+ |\eta| (1+y), \quad y \in (0, \varepsilon^{-2/3}) \\ |\chi(y)| \leq C_- |\eta|, \quad y \in (-\infty, 0). \end{aligned}$$

Two problems in step 2

- We know that the second constraint on ν is satisfied as $y \rightarrow -\infty$:

$$\nu(y) \underset{y \rightarrow -\infty}{\sim} \gamma |y|^{\frac{1-\varepsilon-\xi_\infty^2}{4\varepsilon}} e^{-\frac{|y|}{2\varepsilon^{1/3}}} \Rightarrow \frac{1}{\nu^2(y)} \int_{-\infty}^y \nu^2(s) ds \underset{y \rightarrow -\infty}{\sim} \varepsilon^{1/3}.$$

However, it is hard to justify this constraint for all $y \in (-\infty, 0)$.

- Lipschitz continuity of the mapping $\nu \rightarrow \chi$ is only justified on $(y_0, \varepsilon^{-2/3})$ for an ε -independent $y_0 \in (-\infty, 0)$.

Lemma

Let $\chi_{1,2}$ be defined for $\nu_{1,2} \in L^2(-\infty, \varepsilon^{-2/3}) \cap C^0(-\infty, \varepsilon^{-2/3})$ s.t.

$$\|\nu_{1,2} - \nu_0\|_{L^2(-\infty, \varepsilon^{-2/3})} + \|\nu_{1,2} - \nu_0\|_{L^\infty(-\infty, \varepsilon^{-2/3})} \leq \delta.$$

Then,

$$\|\chi_1 - \chi_2\|_{L^\infty(0, \varepsilon^{-2/3})} \leq C|\eta| \left(\|\nu_1 - \nu_2\|_{L^2(-\infty, \varepsilon^{-2/3})} + \varepsilon^{-1/3} \|\nu_1 - \nu_2\|_{L^\infty(0, \varepsilon^{-2/3})} \right),$$

$$\|\chi_1 - \chi_2\|_{L^\infty(y_0, 0)} \leq C(y_0)|\eta| \left(\|\nu_1 - \nu_2\|_{L^2(-\infty, \varepsilon^{-2/3})} + \|\nu_1 - \nu_2\|_{L^\infty(-\infty, \varepsilon^{-2/3})} \right).$$

Step 3: convergence of the alternating iterations

Let us start the alternating iteration scheme with $\nu = \nu_0$ and define

$$\chi_0(y) = -\frac{\eta}{\nu_0^2(y)} \int_{-\infty}^y \nu_0^2(s) ds.$$

Then, we have $\chi_0 \in C^\infty(\mathbb{R})$ such that

$$\chi_0(y) = -\eta \begin{cases} \frac{1}{2}y + \frac{3}{2}y^{-2} + \mathcal{O}(y^{-5}) & \text{as } y \rightarrow +\infty \\ |y|^{-1/2} + \mathcal{O}(|y|^{-5/4}) & \text{as } y \rightarrow -\infty \end{cases}$$

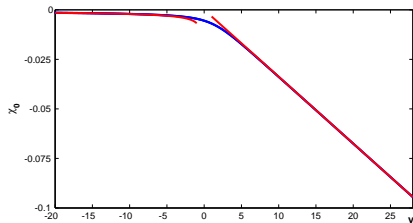
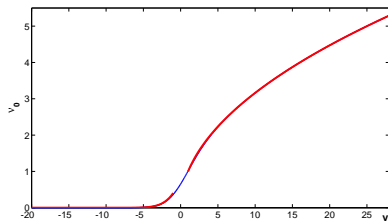


Figure : Components ν_0 (left) and χ_0 (right) for $\eta = \varepsilon$ and $\varepsilon = 0.0067$.

Numerical iteration scheme

Using the mapping $\chi \rightarrow \nu$, we obtain ν_1 from χ_0 . Using the mapping $\nu \rightarrow \chi$, we obtain χ_1 from ν_1 . And so on... The iterations are terminated when the distance between two subsequent approximations is smaller than 10^{-15} .

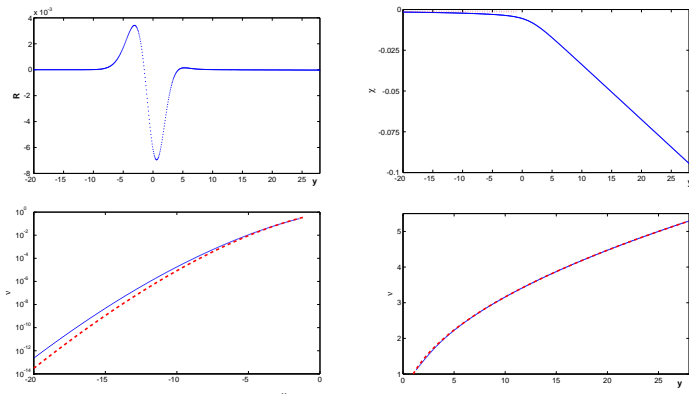


Figure : Component R (top left panel), component χ (top right panel), component ν (bottom panels) in comparison with various asymptotic values shown by dashed lines.

Conclusion

Starting with

$$\varepsilon^2 u''(x) + \left(1 - x^2 - 2i\alpha \varepsilon^{1/2} x - |u(x)|^2\right) u(x) = 0, \quad x \in \mathbb{R}$$

and using

$$u(x) = \varphi(x) e^{\varepsilon^{-1} \int_{-\infty}^x \xi(x') dx'},$$

we considered the Thomas–Fermi limit for the PT-symmetric ground state:

$$\begin{cases} (1 - x^2 - \varphi^2(x) - \xi^2(x)) \varphi(x) = -\varepsilon^2 \varphi''(x), \\ (\varphi^2 \xi)'(x) = 2\eta x \varphi^2(x), \end{cases} \quad x \in \mathbb{R},$$

where $\alpha = \varepsilon^{1/2} \eta$.

We proved existence of the limiting compact state for small η and conjectured on the persistence of the Hastings–McLeod solution for $\eta = \mathcal{O}(\varepsilon^q)$ with $q > \frac{5}{6}$.

Numerical results show the persistence for $\eta = \mathcal{O}(\varepsilon^q)$ with $q \geq 0.2$. Rigorous proof is still opened for further studies...