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ON THE MOUNTAIN-PASS ALGORITHM FOR THE QUASI-LINEAR SCHRÖDINGER EQUATION

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Abstract. We discuss the application of the Mountain Pass Algorithm to the so-called quasi-linear Schrödinger equation, which is naturally associated with a class of nonsmooth functionals so that the classical algorithm cannot directly be used. A change of variable allows us to deal with the lack of regularity. We establish the convergence of a mountain pass algorithm in this setting. Some numerical experiments are also performed and lead to some conjectures.

1. **Introduction and results.** The aim of this paper is to find numerical solutions of mountain pass type for the problem

$$-\Delta u - u\Delta u^2 + Vu = |u|^{p-1}u, \qquad \text{in } \mathbb{R}^N, \tag{1}$$

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for $p > 1$ and $V > 0$. This is the equation of standing waves of the quasi-linear Schrödinger equation

$$\begin{cases} \mathrm{i}\phi_t + \Delta\phi + \phi\Delta|\phi|^2 - V\phi + |\phi|^{p-1}\phi = 0 & \text{in } (0,\infty)\times\mathbb{R}^N, \\ \phi(0,x) = \phi_0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{2}$$

where i stands for the imaginary unit and the unknown $\phi : (0,\infty)\times\mathbb{R}^N \to \mathbb{C}$ is a complex valued function. Various physically relevant situations are described by this quasi-linear equation. For example, it is used in plasma physics and fluid mechanics, in the theory of Heisenberg ferromagnets and magnons and in condensed matter theory, see e.g. the bibliography of [6] and the references therein. The mountain pass solutions of the semi-linear equation $-\Delta u + Vu = |u|^{p-1}u$, corresponding to ground states for the Schrödinger equation

$$\begin{cases} \mathrm{i}\phi_t + \Delta\phi + |\phi|^{p-1}\phi = 0 & \text{in } (0,\infty)\times\mathbb{R}^3, \\ \phi(0,x) = \phi_0(x) & \text{in } \mathbb{R}^3, \end{cases} \tag{3}$$

have been extensively studied in the last decades, both analytically [24] and numerically. On the numerical side, the typical tool is the so-called mountain pass algorithm, originally implemented by Choi and McKenna [4] (see also [2, 3] for a different approach). This works nicely under the assumption that the functional associated with the problem is of class C^1 on a Hilbert space and it satisfies suitable geometrical assumptions. Now, we observe that the functional $\mathcal{E} : X \to \bar{\mathbb{R}}$ naturally but only formally associated with (1) is

$$u \mapsto \mathcal{E}(u) := \frac{1}{2}\int_{\mathbb{R}^N} (1+2u^2)|\nabla u|^2 \,\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^N} Vu^2 \,\mathrm{d}x - \frac{1}{p+1}\int_{\mathbb{R}^N} |u|^{p+1} \,\mathrm{d}x. \tag{4}$$

In fact, taking X as $H^1(\mathbb{R}^N)$ with $N \geq 3$, then the functional (4) is not even well defined, as it might be the case that it assumes the value $+\infty - (+\infty)$ in the range $(N+2)/(N-2) < p < (3N+2)/(N-2)$. In two dimensions, with $X = H^1(\mathbb{R}^2)$, it is well defined from X to $\mathbb{R} \cup \{+\infty\}$ but it is merely lower semi-continuous. If, instead, X stands for the set of $u \in H^1(\mathbb{R}^N)$ such that $u^2 \in H^1(\mathbb{R}^N)$, then it follows that (4) is well defined from X to $\mathbb{R}$, for every choice $1 < p < (3N+2)/(N-2)$. From the physical viewpoint defining X in this way makes it a natural choice for the energy space. On the other hand, for initial data in this space X, currently there is no well-posedness result for problem (2) (see the discussion in [6]). Furthermore, X is not even a vector space, although (X,d) can be regarded as a complete metric space endowed with distance the $d(u,v) = \|u-v\|_{H^1} + \|\nabla u^2 - \nabla v^2\|_{L^2}$ and it turns out that (4) is continuous over (X,d) suggesting that a possible approach to the study of problem (1) could be to exploit the (metric) critical point theory developed in [7]. Nevertheless, this continuity property is not enough to establish the convergence of a traditional Mountain Pass Algorithm. Actually, it is not even clear what a satisfying gradient for $\mathcal{E}$ is. Let us emphasize that we are interested in the convergence of the algorithm in infinite dimensional spaces which ensures the convergence of the discretized problem at a rate which does not blow-up when the mesh used for approximation becomes finer. Hence, in conclusion, neither the mountain pass algorithm can be directly applied for the numerical computation of some solution of (1) nor, to our knowledge, the current literature (see e.g. [15] and the references therein) contains suitable generalization of the mountain pass algorithm to the case of non-smooth functionals, except the case of locally Lipschitz functional, which unfortunately are incompatible with the regularity available for our framework. On the other hand in [5, 6], in order to find the existence and qualitative properties of the solutions to (1), a change of variable procedure was performed to relate the solutions $u \in X$ to (1) with the solutions $v \in H^1(\mathbb{R}^N)$ to an associated semi-linear problem

$$-\Delta v = f(x, v), \qquad f(x, v) := \frac{|r(v)|^{p-1} r(v) - V(x)\, r(v)}{\sqrt{1 + 2r^2(v)}}, \tag{5}$$

where the function $r : \mathbb{R} \to \mathbb{R}$ is the unique solution to the Cauchy problem

$$r'(s) = \frac{1}{\sqrt{1 + 2r^2(s)}}, \qquad r(0) = 0. \tag{6}$$

More precisely, u is a smooth solution (say C^2) to (1) if and only if $v = r^{-1}(u)$ is a smooth solution to (5), that is a critical point of the C^1-functional $\mathcal{T} : H^1(\mathbb{R}^N) \to \mathbb{R}$ defined by

$$v \mapsto \mathcal{T}(v) := \frac{1}{2} \int_{\mathbb{R}^N} |\nabla v|^2 \,\mathrm{d}x - \frac{1}{p+1} \int_{\mathbb{R}^N} |r(v)|^{p+1} \,\mathrm{d}x + \frac{1}{2} \int_{\mathbb{R}^N} V(x)\, |r(v)|^2 \,\mathrm{d}x. \tag{7}$$

In addition, as we shall see, the mountain pass values and the least energy values of these functionals correspond through the function r. Now, by applying the mountain pass algorithm to $\mathcal{T}$, we can find a mountain pass solution v of (5). Then $u = r(v)$ will be a mountain pass solution of the original problem with a reasonable control on numerical errors.

We mention that, at least in the case of large constant potentials V and for a general class of quasi-linear problems, there are some uniqueness results for the solutions, see e.g. [11].

The article is organized as follows. In section 2, we will establish the equivalence between ground state solutions for $\mathcal{E}$ and those for $\mathcal{T}$. Section 3 will recall the mountain pass algorithm and discuss assumptions under which its convergence is guaranteed for our problem. In section 4, we will present our numerical investigations. We finish by a conclusion giving some conjectures and outlining future work.

Notation & terminology. We will denote $\operatorname{Im} f$ the image of a function $f : A \to B$ i.e., $\operatorname{Im} f = \{f(x) : x \in A\}$. The notation $\operatorname{adh}(A)$ stands for the topological closure of the set A. The norm in the Lebesgue spaces $L^p(\Omega)$ will be written $|\cdot|_{L^p(\Omega)}$ (Ω will be dropped if clear from the context). We will call a (nonlinear) *projector* any function that is idempotent i.e., any function f such that $f(x) = x$ for all $x \in \operatorname{Im} f$.

2. **Equivalence between mountain pass values.** We noticed in the introduction that, thanks to the change of unknown $u = r(v)$, solutions $v \in H^1(\mathbb{R}^N) \cap C^2(\mathbb{R}^N)$ to (5) correspond to solutions $u \in X \cap C^2(\mathbb{R}^N)$ to (1) where $X = \{u \in H^1(\mathbb{R}^N) : u^2 \in H^1(\mathbb{R}^N)\}$ (see e.g. [5, 6]). In this section, we want to show that, in addition, if v is at the Mountain Pass level, then u is at the Mountain Pass level too in a suitable functional setting, see formula (10). Hence, numerically computing a Mountain Pass solution v up to a certain error, yields a Mountain Pass solution $u = r \circ v$ to the original problem (1) up to a certain error (involving also the error due to the numerical calculation of the solution r to the Cauchy problem in (6)). In order to prove this, notice that $\mathcal{T} : H^1(\mathbb{R}^N) \to \mathbb{R}$ defined by (7) reads

$$\mathcal{T}(v) = \frac{1}{2} \int_{\mathbb{R}^N} |\nabla v|^2 \,\mathrm{d}x - \int_{\mathbb{R}^N} F(x, v) \,\mathrm{d}x$$

where we have set $F(x,t) := \int_0^t f(x,s)\,\mathrm{d}s$ with f defined by (5). Notice first that, if $u = r(v)$ where $v \in H^1(\mathbb{R}^N) \cap C^2(\mathbb{R}^N)$, then $u \in X \cap C^2(\mathbb{R}^N)$. Furthermore, it follows that

$$\mathcal{E}(u) = \mathcal{T}(v), \tag{8}$$

where $\mathcal{E}$ is the action defined by (4). Indeed, we have

$$\begin{aligned}\mathcal{E}\big(r(v)\big) &= \frac{1}{2}\int_{\mathbb{R}^N} \big(1 + 2r^2(v)\big)(r')^2(v)|\nabla v|^2\,\mathrm{d}x \\ &\qquad - \frac{1}{p+1}\int_{\mathbb{R}^N} |r(v)|^{p+1}\,\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^N} V(x)|r(v)|^2\,\mathrm{d}x \\ &= \frac{1}{2}\int_{\mathbb{R}^N} |\nabla v|^2\,\mathrm{d}x - \frac{1}{p+1}\int_{\mathbb{R}^N} |r(v)|^{p+1}\,\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^N} V(x)\,|r(v)|^2\,\mathrm{d}x \\ &= \mathcal{T}(v),\end{aligned}$$

thanks to the Cauchy problem (6).

Proposition 2.1. *Let $\hat{v} \in H^1(\mathbb{R}^N) \cap C^2(\mathbb{R}^N)$ be a Mountain Pass solution to problem (5), that is*

$$\begin{aligned} &\mathcal{T}(\hat{v}) = \inf_{\gamma\in\Gamma_{\mathcal{T}}} \sup_{t\in[0,1]} \mathcal{T}(\gamma(t)), \\ &\Gamma_{\mathcal{T}} = \big\{\gamma \in C([0,1], H^1(\mathbb{R}^N)) : \gamma(0) = 0,\ \mathcal{T}(\gamma(1)) < 0\big\}. \end{aligned} \tag{9}$$

Then $\hat{u} = r(\hat{v}) \in X \cap C^2(\mathbb{R}^N)$ is a Mountain Pass solution to problem (1), that is

$$\begin{aligned} &\mathcal{E}(\hat{u}) = \inf_{\eta\in\Gamma_{\mathcal{E}}} \sup_{t\in[0,1]} \mathcal{E}(\eta(t)), \\ &\Gamma_{\mathcal{E}} = \big\{\eta \in C([0,1], X) : \gamma(0) = 0,\ \mathcal{E}(\gamma(1)) < 0\big\}. \end{aligned} \tag{10}$$

Furthermore, $\hat{u}$ is also a least energy solution to (1) for the energy $\mathcal{E}$ (i.e., achieving the infimum of $\mathcal{E}$ on non-trivial solutions to (1)).

Proof. It is readily seen that if $\hat{v} \in H^1(\mathbb{R}^N) \cap C^2(\mathbb{R}^N)$ is a solution to (5), then $\hat{u} = r(\hat{v}) \in X \cap C^2(\mathbb{R}^N)$ is a solution to (1). Setting now $\tilde{\Gamma}_{\mathcal{T}} := \{r \circ \gamma : \gamma \in \Gamma_{\mathcal{T}}\}$, on account of (8), we have

$$\mathcal{E}(\hat{u}) = \mathcal{T}(\hat{v}) = \inf_{\gamma\in\Gamma_{\mathcal{T}}} \sup_{t\in[0,1]} \mathcal{T}(\gamma(t)) = \inf_{\tilde{\gamma}\in\tilde{\Gamma}_{\mathcal{T}}} \sup_{t\in[0,1]} \mathcal{E}(\tilde{\gamma}(t)).$$

On the other hand, we will show that $\tilde{\Gamma}_{\mathcal{T}} = \Gamma_{\mathcal{E}}$, yielding assertion (10). In fact, let $\eta \in \Gamma_{\mathcal{E}}$ and consider $\gamma := r^{-1} \circ \eta$. Then, $\eta = r \circ \gamma$ with $\gamma \in C\big([0,1], H^1(\mathbb{R}^N)\big)$, $\gamma(0) = 0$ and $\mathcal{T}(\gamma(1)) = \mathcal{E}(r \circ \gamma(1)) = \mathcal{E}(\eta(1)) < 0$. Hence $\eta \in \tilde{\Gamma}_{\mathcal{T}}$. Vice versa, if $\eta \in \tilde{\Gamma}_{\mathcal{T}}$, there exists $\gamma \in \Gamma_{\mathcal{T}}$ such that $\eta = r \circ \gamma$. Then, it is readily seen that $\eta \in C([0,1], X)$, $\eta(0) = r(\gamma(0)) = r(0) = 0$ and $\mathcal{E}(\eta(1)) = \mathcal{T}(\gamma(1)) < 0$. By Theorem 0.2 of [14], $\hat{v}$ is a least energy solution. In turn, by Step II in the proof of Theorem 1.3 of [5] the last assertion follows. □

Remark 2.2. As we will see in the next section, in our case $f(v)/v$ (where f is defined by (5)) is increasing on $(0, +\infty)$ and therefore mountain pass solutions $\hat{v}$ can be characterized by

$$\mathcal{T}(\hat{v}) = \inf_{v\neq 0} \sup_{t\geq 0} \mathcal{T}(tv)$$

instead of (9). The numerical algorithm described below finds a local minimum $\tilde{v}$ of $v \mapsto \sup_{t\geq 0} \mathcal{T}(tv)$ but there is no absolute guarantee that $\tilde{v}$ is a mountain pass solution. Nonetheless, $\tilde{v}$ is a "saddle point of mountain pass type" [15, Definition 1.2] i.e., there exists an open neighborhood V of $\tilde{v}$ such that $\tilde{v}$ lies in the closure of two path-connected components of $\{v \in V : \mathcal{T}(v) < \mathcal{T}(\tilde{v})\}$. Since the map $v \mapsto r(v) : H^1(\mathbb{R}^N) \to X$ is an homeomorphism and $\mathcal{E}(u) = \mathcal{T}\big(r^{-1}(u)\big)$, the same characterization holds for $\tilde{u} := r(\tilde{v})$. In conclusion, the above discussion can be thought as an extension of the correspondence of proposition 2.1 to saddle point solutions.

3. **Mountain pass algorithms — convergence up to a subsequence.** Let $\mathcal{H}$ be a Hilbert space with norm $\|\cdot\|$, E a closed subspace of $\mathcal{H}$, $\mathcal{T} : \mathcal{H} \to \mathbb{R}$ a $\mathcal{C}^1$-functional and P a peak selection for $\mathcal{T}$ relative to E, i.e., a function

$$P : \mathcal{H} \setminus E \to \mathcal{H} : u \mapsto P(u)$$

such that, for any $u \in \mathcal{H} \setminus E$, $P(u)$ is a local maximum point of $\mathcal{T}$ on $\mathbb{R}^+ u \oplus E = \{tu + e : t \geq 0 \text{ and } e \in E\}$. The Mountain Pass Algorithm (MPA) uses P to perform a constrained steepest descent search in order to find critical points of $\mathcal{T}$. The version we use in this paper is a slightly modified version of the MPA introduced by Y. Li and J. Zhou [16] which in turn is based on the pioneer work of Y. S. Choi and P. J. McKenna [4]. Let us first recall the version of Y. Li and J. Zhou.

Algorithm 3.1 (MPA [16])**.** 1. *Choose an initial guess $u_0 \in \operatorname{Im}(P)$, a tolerance $\varepsilon > 0$ and let $n \leftarrow 0$;*

2. *if $\|\nabla\mathcal{T}(u_n)\| \leq \varepsilon$ then stop;*
otherwise, compute

$$u_{n+1} = P\left(\frac{u_n - s_n \nabla\mathcal{T}(u_n)}{\|u_n - s_n \nabla\mathcal{T}(u_n)\|}\right), \tag{11}$$

for some $s_n \in (0, +\infty)$ satisfying the Armijo's type stepsize condition

$$\mathcal{T}(u_{n+1}) - \mathcal{T}(u_n) < -\frac{1}{2}\|\nabla\mathcal{T}(u_n)\|\|u_{n+1} - u_n\|;$$

3. *let $n \leftarrow n + 1$ and go to step 2.*

Conditions under which the sequence (u_n) generated by the MPA converges, up to a subsequence, to a critical point of $\mathcal{T}$ on $\operatorname{Im} P$ have been studied [17] in the case $\dim E < \infty$.

In [23], N. Tacheny and C. Troestler proved that, if an additional metric projection on the cone K of non-negative functions is performed at each step of the algorithm, the MPA still converges (at least up to a subsequence) and that the limit of the generated sequence is guaranteed to be a non-negative solution. In that paper, the authors studied a variant of the above algorithm where the update at each step is given by

$$u_{n+1} = P\big(P_K(u_n[s_n])\big) \quad \text{where } u_n[s] := u_n - s\frac{\nabla\mathcal{T}(u_n)}{\|\nabla\mathcal{T}(u_n)\|}, \tag{12}$$

for some $s_n \in S(u_n) \subseteq (0, +\infty)$ with P_K being the metric projector on the cone K i.e., $P_K(u) \in K$ is the unique element $v \in K$ that achieves the infimum $\inf_{v \in K}\|v - u\|$. Notice that, with this formulation, the projector P only needs to be defined on the cone K. The set $S(u_n)$ of admissible stepsizes is defined as follows: first let

$$S^*(u_n) := \big\{s > 0 : \ u_n[s] \neq 0 \text{ and } \mathcal{T}\big(PP_K(u_n[s])\big) - \mathcal{T}(u_n) < -\tfrac{1}{2}s\|\nabla\mathcal{T}(u_n)\|\big\}$$

and then define $S(u_n) := S^*(u_n) \cap \big(\frac{1}{2}\sup S^*(u_n), +\infty\big)$. Note that the right hand side of the inequality to satisfy does not depend on P. Under the following assumptions on the action functional $\mathcal{T}$ and the peak selection P:

(P1) $P : K \setminus \{0\} \to K \setminus \{0\}$ is well defined and continuous;
(P2) $\inf_{u \in \mathrm{Im}(P) \cap K} \mathcal{T}(u) > -\infty$;
(P3) $0 \notin \mathrm{adh}(\mathrm{Im}\, P \cap K)$;
(P4) $\mathcal{T}(P_K(u)) \le \mathcal{T}(u) + o(\mathrm{dist}(u, K))$ as $\mathrm{dist}(u, K) \to 0$;

they prove that the algorithm generates a Palais-Smale sequence in K. Roughly, using a numerical deformation lemma, they show that a step $s_n \in S(u_n)$ exists and that it can be chosen in a "locally uniform" way. The trick is to avoid s_n being arbitrarily close to 0 without being "mandated" by the functional. Let us remark that the definition of $S(u_n)$ is natural (but not the only possible one) to force this stepsize not to be "too small". Then, under some additional compactness condition (e.g. the Palais-Smale condition or a concentration compactness result), they establish the convergence up to a subsequence. If furthermore the solution is isolated in some sense, the convergence of the whole sequence is proved.

Let us also mention that, recently, inspired from the theoretical existence result of A. Szulkin and T. Weth [22], the convergence of the sequence generated by the mountain pass algorithm has been proved (in some cases, up to a subsequence) even when $\dim E = \infty$ and $\Omega = \mathbb{R}^N$ (see [13]).

Let us come back to our problem and verify that assumptions (P1)–(P4) hold for the functional $\mathcal{T}$ given by (7) and the projection P defined as follows: $P(u)$ is the unique maximum point of $\mathcal{T}$ on the half line $\{tu : t > 0\}$.

The autonomous case $-\Delta u - u\Delta u^2 = g(u)$ was studied by M. Colin and L. Jeanjean [5] who proved the existence of a positive solution under the assumptions

(g0) g is locally Hölder continuous on $[0, +\infty)$;
(g1) $\lim_{u\to 0} \frac{g(u)}{u} < 0$;
(g2) $\lim_{u\to+\infty} |g(u)|/u^{(3N+2)/(N-2)} = 0$ when $N \ge 3$ or,
for any $\alpha > 0$, there exists $C_\alpha > 0$ such that, for all $u \ge 0$, $|g(u)| \le C_\alpha\, \mathrm{e}^{\alpha u^2}$ when $N = 2$;
(g3) $\exists \psi > 0$ such that $G(\psi) > 0$ where $G(u) := \int_0^u g(t)\,\mathrm{d}t$ when $N \ge 2$ (or $G(\psi) = 0$, $g(\psi) > 0$ and $G(u) < 0$ and $u \in (0, \psi)$ when $N = 1$).

In our case, this situation corresponds to $V \ne 0$ constant and $g(u) = |u|^{p-1}u - Vu$ where assumptions (g0)–(g3) are verified when $p \in \left(3, \frac{3N+2}{N-2}\right)$.

Let us now work with the equivalent problem $-\Delta v = r'(v)g(r(v))$ where r is defined as in the introduction and g verifies (g0)–(g3). Let us call $f(v) := r'(v)g(r(v))$. Recalling that $r(v) \sim v$ when $v \to 0$ and $r(v) \sim \sqrt{v}$ when $v \to +\infty$ [5], (g1) implies that f verifies $\lim_{v\to 0} \frac{f(v)}{v} < 0$. Moreover, as a consequence of (g2), f is subcritical with respect to the critical Sobolev exponent $\frac{N+2}{N-2}$. Therefore $\mathcal{T}$ is well defined on $H^1(\mathbb{R}^N)$ and 0 is a local minimum of $\mathcal{T}$. This establishes (P2)–(P3). Because of (g3) there exists a v^* such that $\mathcal{T}(v^*) < 0$ but, in order to have (P1) and (P4), we need to replace (g3) with the following stronger assumptions (see [23]):

(g4) $F(v)/v^2 \to +\infty$ when $v \to +\infty$ where $F(v) := \int_0^v f(s)\,\mathrm{d}s$;
(g5) $v \mapsto f(v)/v$ is increasing on $(0, +\infty)$.

Let us remark that when the domain is bounded (as in numerical experiments), it is enough to require $\lim_{u\to 0} \frac{f(u)}{u} \le 0$ instead of $\lim_{u\to 0} \frac{f(u)}{u} < 0$. So we can work with $V = 0$ in this case.

For our problem (5) with $V \ne 0$ constant, it is easy to see that (g4) is satisfied. Let us now show that property (g5) holds for $p \ge 3$. First, let us remark that the derivative of $v \mapsto r^k(v)/\big(v\sqrt{1+2r^2(v)}\big)$ is a positive function times

$$\big(k + 2(k-1)r^2\big)(r' \cdot v) - \big((1+2r^2) \cdot r\big). \tag{13}$$

For $k = 1$, this quantity becomes $r'v - (1+2r^2)r$ which is negative because $r'(v) \cdot v \le r$ (see e.g. [5, Lemma 2.2]). Thus the map $v \mapsto -Vr(v)/\big(v\sqrt{1+2r^2(v)}\big)$ is increasing. As a consequence, it remains to prove that $f(v)/v$ is increasing when $V = 0$. For this, it is enough to show that (13) is positive for $k = p$. Using the inequality $r'(v) \cdot v \ge \frac{1}{2} r$ (see e.g. [5, Lemma 2.2]), one readily proves the assertion.

The above arguments imply that the mountain pass algorithm applied to $\mathcal{T}$ generates a Palais-Smale sequence when $3 < p < \frac{3N+2}{N-2}$. Numerically, it is natural to "approximate" the entire space by large bounded domains Ω_R that are symmetric around 0. In the numerical experiments, we will consider $\Omega_R = (-R/2, R/2)^N$. On Ω_R, the Palais-Smale condition holds and consequently the MPA converges up to a subsequence. This approximation is reasonable for two reasons. First, the solution $v(x)$ on $\mathbb{R}^N$ goes exponentially fast to 0 when $|x| \to \infty$. Second, if we consider a family of solutions (v_R) on Ω_R which is bounded and stays away from 0 and we extend u_R by 0 on $\mathbb{R}^N \setminus \Omega_R$, we will now sketch an argument showing that (v_R) converges up to a subsequence to a non-trivial solution on $\mathbb{R}^N$ (see also [8] where authors prove that, for some semilinear elliptic equations $-\Delta v + Vv = f(x, v)$, ground state solutions on large domains weakly converge to a solution on $\mathbb{R}^N$). The boundedness ensures that, taking if necessary a subsequence, $v_R \rightharpoonup v$. At this point, it may well be that $v = 0$. Nevertheless, E. Lieb [18] proved that if a family of functions (v_R) is bounded away from zero in $H^1(\mathbb{R}^N)$ then there exists at least one family $(x_R) \subseteq \mathbb{R}^N$ such that $v_R(\cdot - x_R) \rightharpoonup v^* \ne 0$ up to a subsequence. To conclude that $v^* \ne 0$, it suffices for example to pick up x_R so that $\int_{B(x_R,1)} |v_R|^2 \,\mathrm{d}x \not\to 0$. Intuitively, the role of x_R is to bring back (some of) the mass that v_R may loose at infinity. It is then classical to prove that v^* is a non-trivial solution on $\mathbb{R}^N$. If moreover (v_R) is a family of ground states, no mass can be lost at infinity and so $v_R(\cdot - x_R) \to v^*$. In this case, v^* is a ground state of the problem on $\mathbb{R}^N$. Of course, if (x_R) is bounded in $\mathbb{R}^N$ then $v_R(\cdot - \tilde{x}_R)$ weakly converges to a translation of v^* for any bounded family $(\tilde{x}_R)$. In particular, for $\tilde{x}_R = 0$, v_R weakly converges, up to a subsequence, to a non-trivial solution v. By regularity, $v_R \to v$ in $C^1_{\mathrm{loc}}(\mathbb{R}^N)$ up to a subsequence.

As the moving plane method can be applied to the autonomous case (see [20]), the positive solutions v_R are even w.r.t. each hyperplane $x_i = 0$ and are decreasing in each direction x_i from $x_i = 0$ to $x_i = \pm R$. As (v_R) is bounded away from 0, the mass of v_R is located around 0. Thus v_R converges up to a subsequence to a non-zero positive solution of (5) on $\mathbb{R}^N$. Moreover, it is expected that the ground state solutions are unique, up to a translation, which would imply the convergence of the whole family (v_R). This uniqueness result has been proved for V sufficiently large (see [11]).

The above reasoning can be applied to the sequence generated by the MPA. In Section 4, the numerical experiments will provide bounded families (v_R) of positive (approximate) solutions on Ω_R which are bounded away from zero (when $V \ne 0$). Thus they converge to a solution on $\mathbb{R}^N$ as $R \to \infty$.

For the non-autonomous case (V non-constant), M. Colin and L. Jeanjean [5] proved the existence of a positive solution for the equation $-\Delta u - u\Delta u^2 + V(x)u = g(u)$ on $\mathbb{R}^N$ when

(V1) there exists $V_0 > 0$ such that $V(x) > V_0$ on $\mathbb{R}^N$;
(V2) $\lim_{|x|\to+\infty} V(x) =: V_\infty \in \mathbb{R}$ and $V(x) \le V_\infty$ on $\mathbb{R}^N$;
(g1′) $g(0) = 0$ and g is continuous;
(g2′) $\lim_{u\to 0} \frac{g(u)}{u} = 0$;
(g3′) there exists $p < \infty$ when $N = 1, 2$ or $p < (3N + 2)/(N - 2)$ if $N \ge 3$ and $C > 0$ such that $|g(u)| \le C(1 + |u|^p)$ for any $u \in \mathbb{R}$.
(g4′) $\exists \mu > 4$ such that $0 < \mu G(u) \le g(u)u$ for any $u > 0$ where $G(u) := \int_0^u g(t)\,\mathrm{d}t$.

These assumptions are clearly satisfied for our model nonlinearity $g(u) = |u|^{p-1}u$ with $3 < p < \frac{3N+2}{N-2}$. As before, to prove that $\mathcal{T}$ possesses the properties (P1)–(P4), we need to replace (g4′) with a slightly stronger assumption, namely that $v \mapsto f(x, v)/v$ is increasing on $(0, +\infty)$ for almost every $x \in \mathbb{R}^N$ where f is defined by (5). Essentially repeating the arguments that we developed for the autonomous case, one can show that this assumption is statisfied for our model problem. As a consequence, the MPA generates a Palais-Smale sequence. Since the Palais-Smale condition holds for the ground state level (even on $\mathbb{R}^N$ when V is non-constant), the MPA sequence converges up to a subsequence to a solution of (5).

Concerning the approximation of $\mathbb{R}^N$ by large domains, we can argue similarly to the autonomous case. Numerically (see Section 4.4), (v_R) is bounded away from zero and the peaks of v_R are located around local minimums of V. So, the entire mass of v_R is not going to infinity. Thus, as in the autonomous case, $v_R \to v$ in C^1_{loc} with v being a non-trivial solution on $\mathbb{R}^N$.

4. **Numerical experiments.** In this section, we compute ground state solutions to problem (1) using algorithm 3.1 with the update step (12) (instead of (11)) on problem (5). The algorithm relies at each step on the finite element method. Let us remark that approximations are saddle points of the functional but, as the algorithm is a constrained steepest descent method, it is not guaranteed that they are gound state solutions. Nevertheless, no non-trivial solutions with lower energy have been found numerically.

Let us now give more details on the computation of various objects intervening in the procedure. As we already motivated above, the numerical algorithm will seek solutions v to (5) on a "large" domain $\Omega_R := (-R/2, R/2)^2$ with zero Dirichlet boundary conditions instead of the whole space $\mathbb{R}^2$. Functions of $H^1_0(\Omega_R)$ will be approximated using P^1-finite elements on a Delaunay triangulation of Ω_R generated by Triangle [21]. The matrix of the quadratic form $(v_1, v_2) \mapsto \int_{\Omega_R} \nabla v_1 \nabla v_2$ is readily evaluated on the finite elements basis. A quadratic integration formula on each triangle is used to compute $v \mapsto -\frac{1}{p+1}\int_{\Omega_R} |r(v)|^{p+1}\,\mathrm{d}x + \frac{1}{2}\int_{\Omega_R} V(x)\,|r(v)|^2\,\mathrm{d}x$. The function r is approximated using a standard adaptive ODE solver. The gradient $g := \nabla\mathcal{T}(v)$ is computed in the usual way: the function $g \in H^1_0(\Omega_R)$ is the solution of the equation $\forall\varphi \in H^1_0$, $(g|\varphi)_{H^1_0} = \mathrm{d}\mathcal{T}(v)[\varphi]$ or, equivalently, g is the solution of the following linear equation

$$\begin{cases} -\Delta g = -\Delta v - f(x, v) & \text{in } \Omega_R, \\ g = 0 & \text{on } \partial\Omega_R, \end{cases}$$

where f is defined in (5). This equation is solved using the finite element method.

Since in our case $E = \{0\}$, the projector $P(u)$ is easily computed for any $u \ne 0$: first we pick a $t_1 > 0$ large enough so that $\mathcal{T}(t_1u) \le 0$ and then we use Brent's method to obtain the point at which $t \mapsto \mathcal{T}(tu)$ achieves its maximum in $[0, t_1]$ (alternatively, one could seek t such that $\mathrm{d}\mathcal{T}(tu)[u] = 0$). The stepsize s_n of (12) is determined as follows: we use Brent's method to compute a value of s minimizing $[0,1] \to \mathbb{R} : s \mapsto \mathcal{T}\big(P(P_K(u_n[s]))\big)$. This choice guarantees that no arbitrary small steps are taken unless required by the functional geometry.

The starting function for the MPA is always $(x_1, x_2) \mapsto \big(0.25 - (x_1/R)^2\big)\big(0.25 - (x_2/R)^2\big)$. The program stops when the gradient of the energy functional at the approximation has a norm less than 10^{-2}. Every 100 iterations of the MPA or when it completes, the approximate solution is further improved using a few iterations of Newton's method. Newton's result is rejected if it does not lead to a sufficient improvement of the solution (e.g., in the worse case, Newton's method does not converge). A simple adaptive mesh refinement is also performed in order to increase accuracy while keeping the cost reasonable. The final mesh is required to have at least 3000 nodes (sometimes more when the peak is very localized).

4.1. **Zero potential.** To start, we study the problem

$$-\Delta u - u\Delta u^2 = |u|^{p-1}u \tag{14}$$

in the open bounded domain $(-0.5, 0.5)^2$. Running the mountain pass algorithm with $p = 4$ and $R = 1$, we get the results presented in Fig. 1 and Table 1. The number of iterations is about 20, except for $R = 1$ where it is 198, presumably because the final iterate is distant from the initial function. These experiments suggest that the solutions go to 0 as $R \to \infty$, that is when balls become larger. This is not surprising. Indeed, for $N \geq 2$, the classical Pohǒzaev identity for the semi-linear problem $-\Delta v = f(v)$ on $\mathbb{R}^N$ reads

$$\int_{\mathbb{R}^N} \Big[\frac{N-2}{2} f(v)v - NF(v)\Big]\, \mathrm{d}x = 0 \tag{15}$$

where F is the primitive of f with $F(0) = 0$. In our case, f is given by eq. (5) with $V = 0$ and thus $F(v) = |r(v)|^{p+1}/(p+1)$. Hence for instance for $N = 2$, the condition (15) becomes

$$\int_{\mathbb{R}^2} |r(v)|^{p+1} = 0.$$

Thus $r(v) = 0$ or, equivalently, $v = 0$.

We also repeat the experiments with the larger exponent $p = 6$ i.e., we consider the problem:

$$-\Delta u - u\Delta u^2 = |u|^5 u. \tag{16}$$

The same conclusions can be drawn in this case.

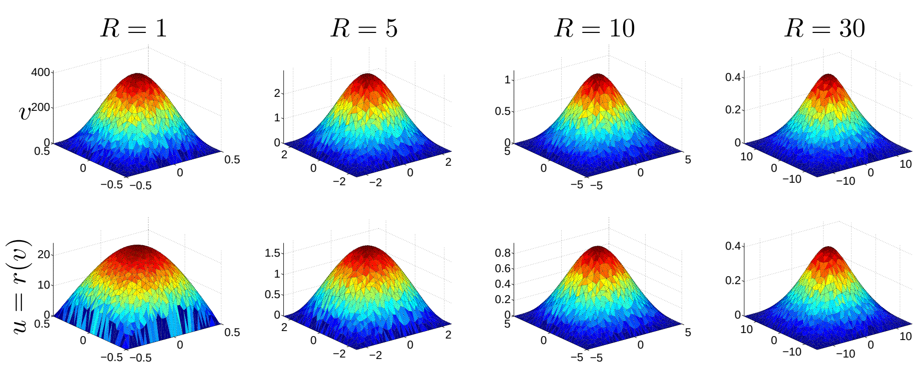

FIGURE 1. Sol. v to (5) and $u = r(v)$ to (1) on Ω_R for $V = 0$ and $p = 4$.

	$R=1$	$R=5$	$R=10$	$R=30$
$\max v$	415.8	2.97	1.17	0.45
$\lvert\nabla v\rvert_{L^2}$	875	5.89	2.19	0.80
$\max u$	24.2	1.77	0.94	0.42
$\mathcal{T}(v)=\mathcal{E}(u)$	78148	6.75	1.19	0.18
$\lVert\nabla\mathcal{T}(v)\rVert$	$8.2\cdot 10^{-8}$	$1.4\cdot 10^{-11}$	$1.6\cdot 10^{-10}$	$9.6\cdot 10^{-10}$
# iter	198	22	18	24

TABLE 1. Characteristics of approximate solutions v to (5) and $u=r(v)$ to (1) on Ω_R for $V=0$ and $p=4$.

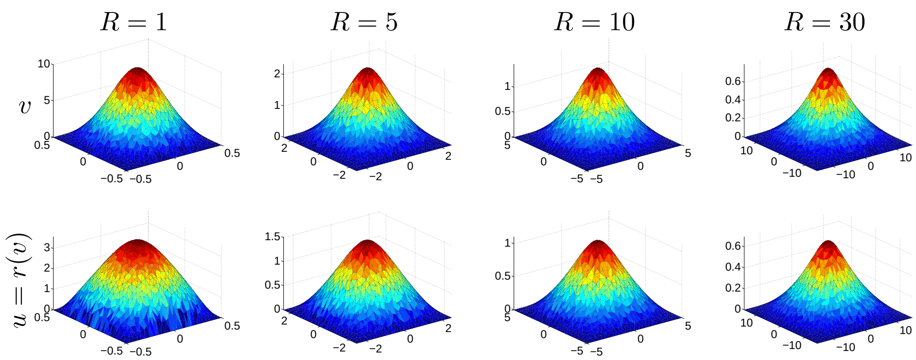

FIGURE 2. Sol. v to (5) and $u=r(v)$ to (1) on Ω_R for $V=0$ and $p=6$.

	$R=1$	$R=5$	$R=10$	$R=30$
$\max v$	10.10	2.34	1.46	0.80
$\lvert\nabla v\rvert_{L^2}$	18.96	4.15	2.52	1.32
$\max u$	3.59	1.52	1.11	0.70
$\mathcal{T}(v)=\mathcal{E}(u)$	87.5	5.00	1.97	0.58
$\lVert\nabla\mathcal{T}(v)\rVert$	$2\cdot 10^{-8}$	$4.2\cdot 10^{-11}$	$3\cdot 10^{-8}$	$2\cdot 10^{-9}$
# iter	28	22	25	25

TABLE 2. Characteristics of approximate solutions v to (5) and $u=r(v)$ to (1) on Ω_R for $V=0$ and $p=6$.

Then, for p in the range $[4,7]$, on Fig. 3, we compare the energies and the L^∞-norms of the mountain pass approximation given previously (our problem with $V=0$) with those of the approximation of the problem $-\Delta u=|u|^{p-1}u$. Equation (14) and the latter one are particular cases of the following family. Let $r_\delta:\mathbb{R}\to\mathbb{R}$ be the unique solution of the Cauchy problem

$$r_\delta'(s)=\frac{1}{\sqrt{1+\delta r^2(s)}},\qquad r_\delta(0)=0.$$

If v is a solution of (5) with $r=r_\delta$, then $u=r_\delta(v)$ is a solution to (1) for $\delta=2$ and to the Lane-Emden equation for $\delta=0$. On Figure 3, we have in addition draw the curve for $\delta=1$ to shed some light on this homotopy.

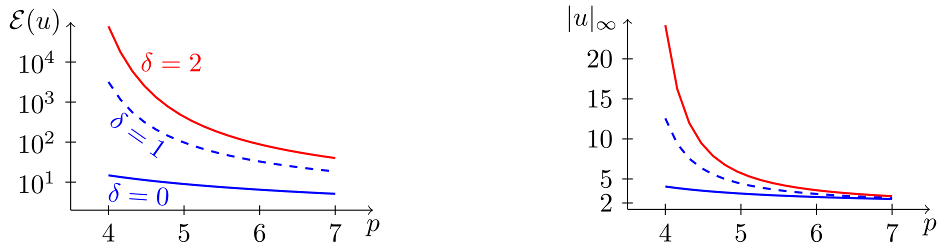

FIGURE 3. Comparison between (1) with $V = 0$ and the problem $-\Delta u = |u|^{p-1}u$ on $(-0.5, 0.5)^2$.

4.2. **Non-zero potentials.** In this section, we study the case $V = 10$ and $p = 4$ or 6. We repeat the experiments above, see Figures 4 and 5 as well as Tables 3 and 4. As before, we also compare the energies and the L^∞-norms of the mountain pass approximation given previously (our problem with $V = 10$) with those of the approximation of the problem $-\Delta u + 10u = |u|^{p-1}u$ for $p \in [4, 7]$, see Fig. 6. To explain that the number of iterations quickly becomes large as R increases, one must remember that one approximates a problem on $\mathbb{R}^N$ which is translation invariant and thus possesses a continuum of solutions. Thus the solution becomes closer to a degenerate one as R increases, implying that the MPA — a constrained steepest descent method — is slow and that Newton's method often fails to converge (and thus its output is rejected).

Contrarily to section 4.1, when $R \to \infty$, the solutions no longer vanish but seem to converge to a non-trivial positive solution on $\mathbb{R}^N$. This is what is expected in view of the argumentation in section 3.

We conclude this section by examining the behavior of the solutions as the potential V goes to 0. Figure 7 depicts the energy of the solution to (1) obtained by the Mountain Pass Algorithm on Ω_R with $R = 10$ for various values of V. It clearly suggests that $\mathcal{E}(u) \to 0$ as $V \to 0$, indicating that the ground-state solutions bifurcate from 0 as V approaches the bottom of the spectrum.

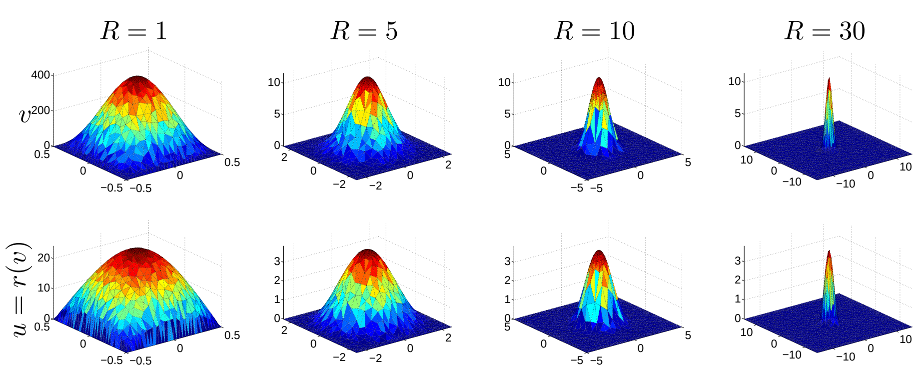

FIGURE 4. Sol. v to (5) and $u = r(v)$ to (1) on Ω_R for $V = 10$ and $p = 4$.

4.3. **Exponential nonlinearity.** Since our numerical experiments are performed in two dimensions, it is natural to wonder what shape the solutions are expected to have when the nonlinearity has exponential growth. To that aim, we consider in

	$R = 1$	$R = 5$	$R = 10$	$R = 30$
$\max v$	417	11.6	11.6	11.6
$\lvert\nabla v\rvert_{L^2}$	877	20.9	20.8	20.8
$\max u$	24.24	3.87	3.87	3.87
$\mathcal{T}(v) = \mathcal{E}(u)$	79183	217	217	216.7
$\lVert\nabla\mathcal{T}(v)\rVert$	$2 \cdot 10^{-8}$	$4 \cdot 10^{-10}$	$2 \cdot 10^{-8}$	$1.6 \cdot 10^{-8}$
# iter	210	43	800	1125

TABLE 3. Characteristics of approximate solutions v to (5) and $u = r(v)$ to (1) on Ω_R for $V = 10$ and $p = 4$.

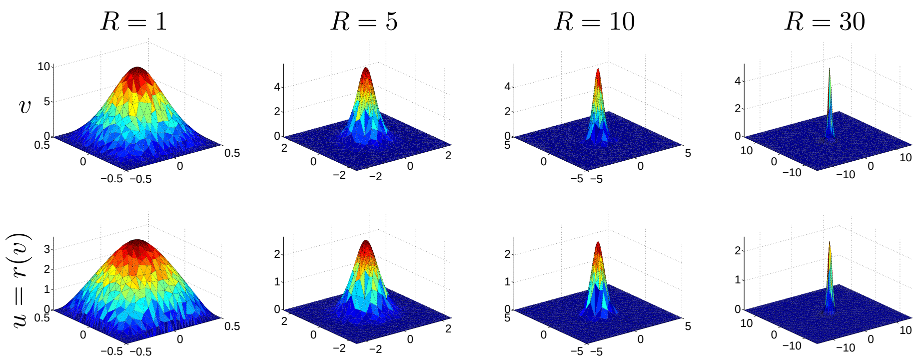

FIGURE 5. Sol. v to (5) and $u = r(v)$ to (1) on Ω_R for $V = 10$ and $p = 6$.

	$R = 1$	$R = 5$	$R = 10$	$R = 30$
$\max v$	10.57	5.98	5.98	5.98
$\lvert\nabla v\rvert_{L^2}$	19.56	9.73	9.73	9.72
$\max u$	3.68	2.68	2.68	2.68
$\mathcal{T}(v) = \mathcal{E}(u)$	105.1	47.3	47.3	47.3
$\lVert\nabla\mathcal{T}(v)\rVert$	$7 \cdot 10^{-12}$	$8.8 \cdot 10^{-9}$	$5.6 \cdot 10^{-8}$	$1.2 \cdot 10^{-8}$
# iter	26	903	1000	863

TABLE 4. Characteristics of approximate solutions v to (5) and $u = r(v)$ to (1) on Ω_R for $V = 10$ and $p = 6$.

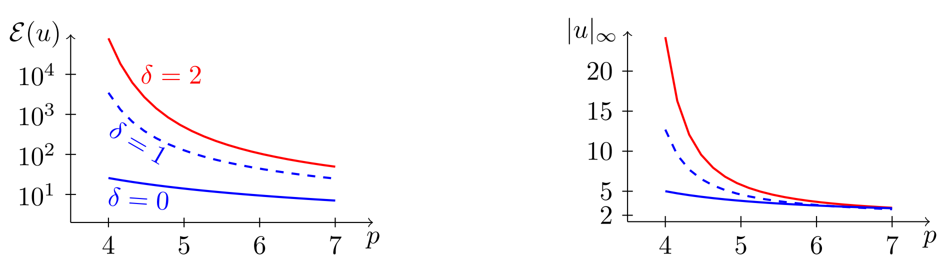

FIGURE 6. Comparison between (1) with $V = 0$ and the problem $-\Delta u + 10u = |u|^{p-1}u$ on $(-0.5, 0.5)^2$.

this section the equation

$$- \Delta u - u\Delta u^2 + Vu = \exp(u^2) - 1. \tag{17}$$

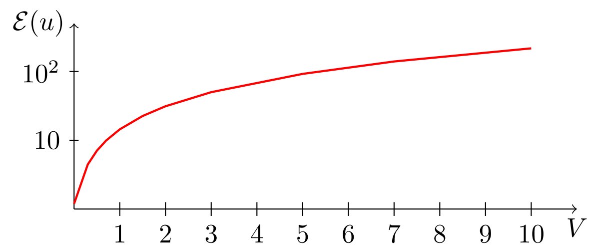

FIGURE 7. Energy of the solutions to (1) on Ω_{10} as $V \to 0$.

The outcome of the numerical computations is presented on Figures 8–9 and Tables 5–6. For $R = 30$, the MPA was started with an initial mesh that was refined in the center of Ω to improve its convergence. Unsurprisingly, one may see that the qualitative behavior of the solutions is similar to what could be observed before with power nonlinearities.

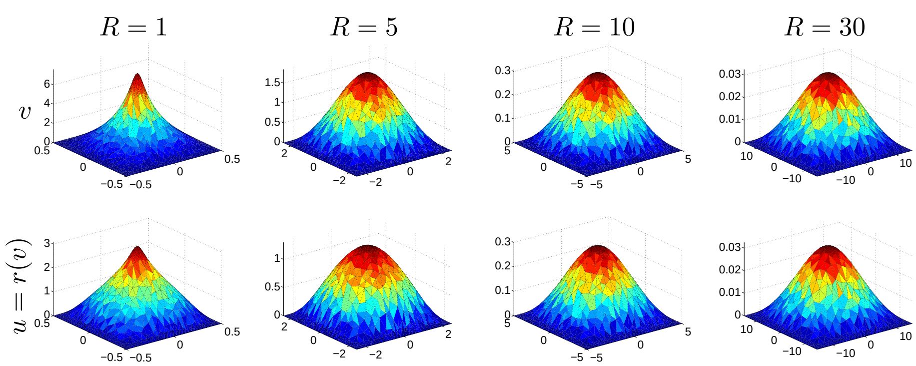

FIGURE 8. Sol. to (17) on Ω_R for $V = 0$.

	$R = 1$	$R = 5$	$R = 10$	$R = 30$
$\max v$	7.6	1.85	0.31	0.03
$\lvert\nabla v\rvert_{L^2}$	11	3.76	0.63	0.065
$\max u$	3.1	1.30	0.30	0.03
$\mathcal{T}(v) = \mathcal{E}(u)$	44.4	2.02	0.06	0.0007
$\lVert\nabla \mathcal{T}(v)\rVert$	$3 \cdot 10^{-8}$	$7 \cdot 10^{-11}$	$1.7 \cdot 10^{-7}$	$1.3 \cdot 10^{-9}$
# iter	28	18	21	21

TABLE 5. Characteristics of approximate solutions v and $u = r(v)$ to (17) on Ω_R for $V = 0$.

4.4. **Non-constant potentials.** To conclude this investigation, let us examine the case of a variable potential. E. Gloss [12] in dimension $N \geq 3$ and J. M. do Ó and U. Severo [9] for $N = 2$ showed that the equation

$$-\varepsilon^2(\Delta u + u\Delta u^2) + V(x)u = g(u) \quad \text{in } \mathbb{R}^N \tag{18}$$

possesses solutions concentrating around local minima of the potential V when $\varepsilon \to 0$. When the potential is constant, this corresponds to $R = 1/\varepsilon$ and, for a

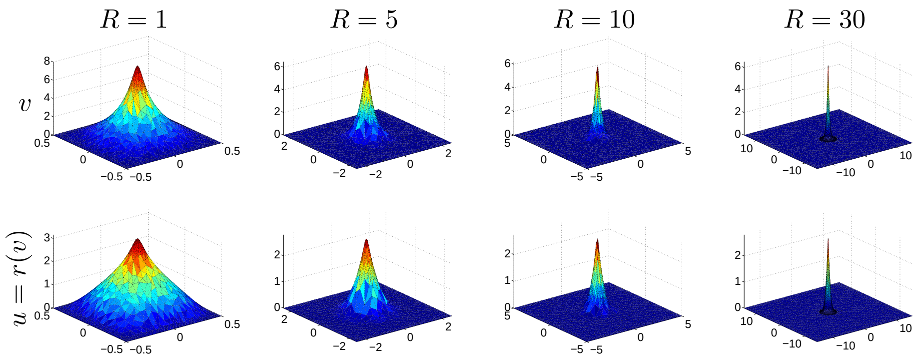

FIGURE 9. Sol. to (17) on Ω_R for $V = 10$.

	$R = 1$	$R = 5$	$R = 10$	$R = 30$
$\max v$	8.04	6.63	6.63	6.62
$\lvert\nabla v\rvert_{L^2}$	10.98	9.10	9.10	9.09
$\max u$	3.17	2.84	2.84	2.84
$\mathcal{T}(v) = \mathcal{E}(u)$	50.60	41.47	41.45	41.31
$\lVert\nabla\mathcal{T}(v)\rVert$	$3.6 \cdot 10^{-7}$	$8.6 \cdot 10^{-8}$	$8.5 \cdot 10^{-9}$	$4.3 \cdot 10^{-8}$
# iter	30	600	800	631

TABLE 6. Characteristics of the approximate solutions v and $u = r(v)$ to (17) for $V = 10$.

positive potential, the above graphs show a concentration around the origin on a bounded domain (which suggests that any point will do on $\mathbb{R}^N$). In this section we have considered (18) on $(-0.5, 0.5)^2$ with $g(u) = |u|^3 u$ and the double well potential

$$V(x) := 10 - 8\exp\bigl(-20\,|x - c|^2\bigr) - 5\exp\bigl(-30\,|x - c'|^2\bigr)$$

where $c = (-0.2, 0.2)$ and $c' = (0.3, -0.2)$. It is pictured on Fig. 10. Note that the two wells have different depths. For $\varepsilon = 0.05$, the MPA returns two different solutions (see Fig. 10) depending on the initial function. (We have chosen not to display the function v as its shape is similar to the one of u.) The left solution u_1, located around the lower well of V, has the lower energy value: $\mathcal{E}(u_1) \approx 0.11$. It is obtained by using the MPA with the same initial guess as before. For the right one u_2, the MPA is applied starting with a function localized at the other well, namely

$$(x_1, x_2) \mapsto \max\bigl\{0,\ 0.1 - (x_1 - c_1')^2 - (x_2 - c_2')^2\bigr\}. \tag{19}$$

It has a higher energy: $\mathcal{E}(u_2) \approx 0.26$. For larger ε, such as $\varepsilon = 0.25$, the MPA returns only one solution with a maximum point not too far from the point at which V achieves its global minimum, see the rightmost graph on Fig. 10 (the graph depicted is the outcome of the MPA with the usual initial function but even using the function (19) as a starting point gives the same output). For even larger ε, such as $\varepsilon = 1$, the solution is very similar to the one for $R = 1$ displayed on Fig. 4.

5. **Conclusion.** In this paper, we tackled the computation of ground state solutions for a class of quasi-linear Schrödinger equations which are naturally associated with a non-smooth functional. A change of variable was used to overcome the lack

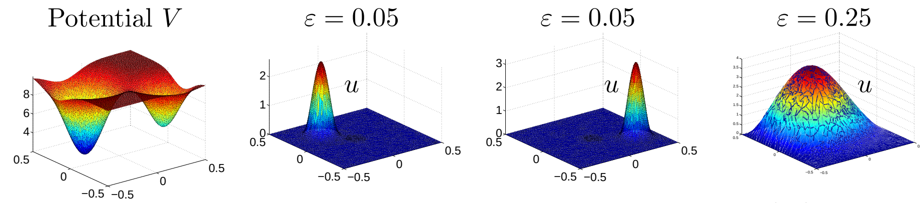

FIGURE 10. Potential V and the corresponding sol. u to (18) on $(-0.5, 0.5)^2$ for $p = 4$.

of regularity and a mountain pass algorithm was applied to the resulting functional to compute saddle point solutions.

In the autonomous case, we outlined arguments and saw on the above numerical computations that the numerical solution u_R on Ω_R converges to a radially symmetric solution u^* on the whole space as $R \to \infty$. The existence of u^* was proved by Colin and Jeanjean [5]. The fact that the same numerical solution is found with many different initial guesses suggests that the ground state solution on $\mathbb{R}^N$ is unique, a fact that was proved [11] for V large. The numerical computations also suggest that ground state solutions u_V^* (where the dependence on V has been made explicit) bifurcate from 0 as $V \to 0$.

For the case of variable potential, the numerical computations exhibited the existence of several solutions of mountain pass type which are local minima of the functional $\mathcal{T}$ on the peak selection set $\operatorname{Im} P$. The asymptotic profile of these solutions seems to be radial (up to a suitable translation) as it is expected from the theoretical results on $\mathbb{R}^N$ for $\varepsilon \to 0$ [12, 9]. Interestingly, the multiplicity of positive solutions does not seem to persist when ε grows larger. Whether the multiple solutions come through a bifurcation from the branch of ground state solutions as ε goes to 0 may be the subject of future investigations.

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