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# Existence, multiplicity and profile of sign-changing clustered solutions of a semiclassical nonlinear Schrödinger equation

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#### Abstract

We study the existence and multiplicity of sign-changing solutions for the Dirichlet problem

 $\begin{cases} -\varepsilon^2 \Delta v + V(x)v = f(v) & \text{in } \Omega, \\ v = 0 & \text{on } \partial \Omega, \end{cases}$ 

where  $\varepsilon$  is a small positive parameter,  $\Omega$  is a smooth, possibly unbounded, domain, f is a superlinear and subcritical nonlinearity, V is a positive potential bounded away from zero. No symmetry on V or on the domain  $\Omega$  is assumed. It is known by Kang and Wei (see [X. Kang, J. Wei, On interacting bumps of semiclassical states of nonlinear Schrödinger equations, Adv. Differential Equations 5 (2000) 899–928]) that this problem has positive *clustered* solutions with peaks approaching a local maximum of V. The aim of this paper is to show the existence of *clustered* solutions with mixed positive and negative peaks concentrating at a local minimum point, possibly degenerate, of V.

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## 1. Introduction

Let us consider the following nonlinear perturbed elliptic equation

$$-\varepsilon^2 \Delta v + V(x)v = |v|^{p-2}v \quad \text{in } \Omega$$

where  $\Omega$  is a smooth domain in  $\mathbb{R}^N$ ,  $N \ge 2$ ,  $V \in \mathscr{C}^1(\Omega, \mathbb{R})$  is bounded from below away from zero, the exponent p satisfies  $2 for <math>N \ge 3$  and p > 2 for N = 2. Equations of this kind arise in different models. For example, the solutions of (1.1) can be regarded as the stationary states of the following nonlinear Schrödinger equation

$$i\varepsilon \frac{\partial \psi}{\partial t} = -\varepsilon^2 \Delta \psi + V(x)\psi - |\psi|^{p-2}\psi.$$

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Eq. (1.1) has been widely studied in many aspects: a large number of papers have been devoted in investigating the existence, multiplicity and asymptotic behavior of positive solutions in the semiclassical limit  $\varepsilon \to 0^+$ . There are many results establishing solutions which exhibit sharp peaks near a certain number of points and vanish everywhere else. It turns out that while least energy solutions develop a single peak, looking for higher energy solutions multiple peaks are found.

If  $\Omega = \mathbb{R}^N$ , then concentration occurs at the critical points of *V*. The first result has been obtained by Floer and Weinstein [20] in the one-dimensional case. Later this line of research has been extensively pursued in a set of recent papers (we recall, among many others, [2,4,15,16,29,38,39], see [3] for further references) obtaining single and multiple peaks at separate critical points, possibly degenerate, of *V*. In particular, we point out the result by Kang and Wei [28] where a new kind of solution is found, the so called *cluster*, i.e. a combination of several interacting peaks concentrating at the same point as  $\varepsilon \to 0^+$ ; the result reads as: given  $K \ge 1$  and  $P_0$  a strict local maximum of *V*, there exists a solution with *K* peaks concentrating at  $P_0$ . While in all the previous papers the peaks concentrate at separate points, so that the interaction between the peaks is negligible, in this case the concentration point is the same so that the interaction effect cannot be neglected and it contributes to the existence of a *cluster*.

Concerning Eq. (1.1) in bounded domains  $\Omega$  with  $V \equiv 1$  and Neumann boundary conditions, it is known the existence of one or more boundary peaks (i.e. peaks with their maximum point located on the boundary) concentrating at separate critical points of the mean curvature of  $\partial \Omega$  (see, for example, [12,19,24,26,27,30,33,40]). In [12] and [27] the authors prove the corresponding result for the Neumann problem of that by Kang and Wei: in this case the *cluster* consists of *K* boundary peaks and the concentration point is a local minimum of the mean curvature. As regards interior spike solutions, in [23] and [25] multiple interior peaks are constructed and their location is strictly related to the geometry of the domain.

As far as it concerns the Dirichlet problem associated to Eq. (1.1) with  $\Omega$  bounded and  $V \equiv 1$ , we quote the papers [8,13,18,22,32,34,35,41], where single and multiple interior peaks are found: concentration occurs, roughly speaking, at distinct critical points of the distance function from the boundary  $\partial \Omega$ .

All the above results are concerned with positive solutions. While there is a wide literature studying existence, multiplicity and shape of positive solutions, there are few papers dealing with the case of sign-changing solutions, with the exception of the one-dimensional case (see [17]) or the radial case which allows methods, like the use of a natural constraint, which do not work in the nonradial setting considered here. We are only aware of few papers. The first result is due to Noussair and Wei in [36], where the Neumann problem associated to (1.1) with  $V \equiv 1$  is studied and it is proved that for  $\varepsilon$  sufficiently small there exists a solution with one positive boundary peak and one negative boundary peak; moreover such peaks approach the global maximum points of the mean curvature. In the particular case when the set of global maxima consists of a single point, then the peaks concentrate at the same point giving rise to a *cluster*. Recently, in [31] the authors obtain nodal solutions with multiple boundary peaks concentrating at different critical points of the mean curvature. The first paper providing a multiplicity result for sign-changing peak solutions is due to Wei and Weth [42]: they consider the Neumann problem in a two-dimensional domain and prove that, given  $K \ge 1$  and given  $P_0$  a strict local minimum of the mean curvature, there exists a *clustered* solution with K positive boundary peaks and K negative boundary peaks concentrating at  $P_0$ ; moreover the positive and the negative peaks are located alternately on the curve  $\partial \Omega$ .

Existence of nodal solutions for the Dirichlet problem when  $V \equiv 1$  has been established in [37] obtaining two interior peaks (one positive and one negative) at different points of  $\Omega$  whose location depends on the geometry of the domain.

As regards sign-changing peak solutions for Eq. (1.1) in the whole space  $\mathbb{R}^N$ , in [1] double peak nodal solutions are produced near a local minimum of V. Furthermore in [14], under some symmetric assumptions on the potential V, the authors construct *clustered* solutions with an arbitrarily large number of positive and negative peaks which collapse to either a local maximum or a local minimum point of V.

Finally we also mention the papers [6,7,5,9,10], where, by using a different approach, a lower bound on the number of sign-changing solutions is provided; however these papers are not concerned with the shape of such solutions.

As far as we know the question of the existence of *clustered* solutions with mixed positive and negative peaks, without symmetry assumptions on the potential V(x) or on the domain  $\Omega$ , is largely open: the result we present here is a contribution to this matter.

Since we do not want to restrict ourselves to a situation where the nonlinearity in (1.1) is homogeneous, we will consider the more general problem

$$\begin{cases} \varepsilon^2 \Delta v - V(x)v + f(v) = 0 & \text{in } \Omega, \\ v = 0 & \text{on } \partial \Omega, \end{cases}$$
(1.2)

where  $f : \mathbb{R} \to \mathbb{R}$ . Let us now state the hypotheses on the potential V that will be used:

- (V1)  $V \in \mathscr{C}^1(\Omega, \mathbb{R})$  and  $\inf_{\Omega} V > 0$ ;
- (V2) there is an open set  $\Lambda$  compactly contained in  $\Omega$  such that  $V \in \mathscr{C}^2(\Lambda, \mathbb{R})$  and

$$P_0 \in \Lambda$$
,  $V(P) > V(P_0) \quad \forall P \in \Lambda \setminus \{P_0\};$ 

(V3) there exists  $l \ge 2$  such that V is l times differentiable at  $P_0$ ,  $D^j V(P_0) = 0$  for j = 1, ..., l - 1 and  $D^l V(P_0)$  is positive definite.

Our local assumption on the behavior of V at  $P_0$  implies that  $P_0$  is a local minimum point for V with nondegenerate *l*th-derivative. Set  $V_0 = V(P_0)$ . Besides (V1)–(V3), throughout this paper the following additional hypotheses on f will be assumed:

(f1)  $f \in \mathscr{C}_{loc}^{1+\sigma}(\mathbb{R}) \cap \mathscr{C}^2(0, +\infty)$  with  $\sqrt{\frac{3l-2}{l}} - 1 < \sigma < 1$ ; f(0) = f'(0) = 0; f(t) = -f(-t) for all  $t \in \mathbb{R}$ ; (f2) the problem in the whole space

$$\Delta w - V_0 w + f(w) = 0, \quad w > 0 \text{ in } \mathbb{R}^N,$$
  

$$w(0) = \max_{x \in \mathbb{R}^N} w(x), \quad \lim_{|x| \to +\infty} w(x) = 0,$$
(1.3)

has a unique solution w, which is nondegenerate, i.e., denoting by L the linearized operator

$$L: H^2(\mathbb{R}^N) \to L^2(\mathbb{R}^N), \quad L[u]:= \Delta u - V_0 u + f'(w) u$$

then

$$\operatorname{Kernel}(L) = \operatorname{span}\left\{\frac{\partial w}{\partial x_1}, \dots, \frac{\partial w}{\partial x_N}\right\}.$$
(1.4)

By the well-known result of Gidas, Ni and Nirenberg [21] w is radially symmetric and strictly decreasing in r = |x|. Moreover, by classical regularity results, the following asymptotic behavior holds:

$$w(r), \ w''(r) = \frac{A}{r^{(N-1)/2}} e^{-\sqrt{V_0}r} \left(1 + O\left(\frac{1}{r}\right)\right),$$
  

$$w'(r) = -\frac{A}{r^{(N-1)/2}} e^{-\sqrt{V_0}r} \left(1 + O\left(\frac{1}{r}\right)\right),$$
(1.5)

where A > 0 is a suitable positive constant.

The class of nonlinearities f satisfying (f1)–(f2) includes, and it is not restricted to, the model  $f(v) = |v|^{p-2}v$  with p > 2 if N = 1, 2 and  $2 if <math>N \ge 3$ . Other nonlinearities can be found in [11].

The main purpose of this paper is to prove that, given two positive integers h, h' with  $h + h' \leq 6$  (with the exception of the couples (1, 5) and (5, 1) in the two-dimensional case), for  $\varepsilon$  sufficiently small (1.2) possesses a *cluster* with h positive peaks and h' negative peaks approaching  $P_0$ . Furthermore each peak has a profile similar to w suitably rescaled. More precisely we will prove the following result.

**Theorem 1.1.** Assume that  $\Omega \subset \mathbb{R}^N$  is a smooth, possibly unbounded, domain and that hypotheses (V1)–(V3) and (f1)–(f2) hold. Let h, h' satisfying

$$h, h' \ge 1, \quad \ell := h + h' \le 6, \quad (h, h') \ne (1, 5), (5, 1) \quad \text{if } N = 3.$$

Then, for  $\varepsilon > 0$  sufficiently small, the problem (1.2) has a solution  $v_{\varepsilon} \in H_0^1(\Omega)$ . Furthermore there exist  $P_1^{\varepsilon}, \ldots, P_{\ell}^{\varepsilon} \in \Omega$  such that, as  $\varepsilon \to 0^+$ ,

(i) 
$$v_{\varepsilon}(x) = \sum_{i=1}^{h} w(\frac{x - P_i^{\varepsilon}}{\varepsilon}) - \sum_{i=h+1}^{\ell} w(\frac{x - P_i^{\varepsilon}}{\varepsilon}) + o(\varepsilon) \text{ uniformly for } x \in \overline{\Omega};$$
  
(ii)  $|P_i^{\varepsilon} - P_j^{\varepsilon}| \ge (1 + o(1)) \frac{2\varepsilon}{\sqrt{V_0}} \log \frac{1}{\varepsilon} \text{ for } i \neq j \text{ and } P_1^{\varepsilon}, \dots, P_{\ell}^{\varepsilon} \to P_0.$ 

An easy computation shows that we obtain 9 pairs of sign-changing peak solutions for problem (1.2) if  $N \ge 3$  and 8 pairs N = 2 provided that  $\varepsilon$  is small enough.

It is interesting to compare our result with that by Kang and Wei: indeed it is known by [28] that there are no positive *clustered* solutions at the local nondegenerate minimum points of V for Eq. (1.1) in  $\mathbb{R}^N$ . The reason is that, in the present situation, the interplay between the opposite peaks creates a new solution with *clustering* peaks near a minimum  $P_0$ .

The proof of Theorem 1.1 relies on the Lyapunov–Schmidt reduction method, which reduces the problem to finding a critical point for a functional defined on a finite-dimensional space. This procedure has been widely used successfully in literature. To simplify the presentation, we shall postpone the reduction process to the appendices in order to derive quickly the finite-dimensional problem. The reduced functional, up to a constant, has the form

$$M_{\varepsilon}(P_1,\ldots,P_{\ell}) = \sum_{i=1}^{\ell} V(P_i) - \sum_{i \neq j} \lambda_i \lambda_j w\left(\frac{P_i - P_j}{\varepsilon}\right) + \text{h.o.t.}$$

and our solutions will correspond to the critical points of  $M_{\varepsilon}$  on a suitable configuration set, where the unknown  $P_i$  determine the location of the peaks. Here  $\lambda_i = \pm 1$  according to the sign of each peak. The product  $\lambda_i \lambda_j$  determines whether the interaction is repulsive or attractive: indeed  $M_{\varepsilon}$  can be rewritten as

$$M_{\varepsilon}(P_1,\ldots,P_{\ell}) = \sum_{i=1}^{\ell} V(P_i) + \sum_{\lambda_i = -\lambda_j} w\left(\frac{P_i - P_j}{\varepsilon}\right) - \sum_{i \neq j, \, \lambda_i = \lambda_j} w\left(\frac{P_i - P_j}{\varepsilon}\right) + \text{h.o.t.}$$
(1.6)

So the reduced functional  $M_{\varepsilon}$  consists of three main terms: the first term depends on the potential effect, the second term is due to the interplay between opposite peaks and has an attractive effect, the third term is due to the interaction between the peaks of the same sign and has a repulsive effect. Observe that the potential term  $\sum_{i=1}^{\ell} V(P_i)$  decreases when the points  $P_i$  are closed to  $P_0$ , while, using (1.5), the interaction term  $\sum_{\lambda_i = -\lambda_j} w(\frac{P_i - P_j}{\varepsilon})$  decreases when the mutual distance between the points  $P_i$  is big, i.e. when the point  $P_i$  are far away from each other. If the third term  $\sum_{i \neq j, \lambda_i = \lambda_j} w(\frac{P_i - P_j}{\varepsilon})$  was negligible, we could easily conclude that the equilibrium is achieved for a suitable configuration of the points  $P_i$ , which is a local minimum for the functional  $M_{\varepsilon}$ . Unfortunately nothing is a priori known on the size of the term  $\sum_{i \neq j, \lambda_i = \lambda_j} w(\frac{P_i - P_j}{\varepsilon})$ , because we have no a priori information on the location of  $P_i$ , with the exception of symmetric settings. Indeed in [14] when  $\Omega = \mathbb{R}^N$  and V is symmetric it is possible to prove that  $M_{\varepsilon}$  has a local minimum restricted to suitable natural constraints, which allow us to keep away from each other the peaks having the same sign.

In the nonsymmetric case the argument above stops working. In general we have no hope to catch a critical point of  $M_{\varepsilon}$  as a local minimum or a local maximum since we cannot expect that the three terms in (1.6) may balance at some minimum or a maximum configuration. However the different interaction effects provide  $M_{\varepsilon}$  with a suitable local linking structure. The central part of the paper is devoted to provide the three main ingredients to apply a max-min argument to  $M_{\varepsilon}$ : (i) the choice of a family of sets in  $\mathbb{R}^{N\ell}$  which allow to define a suitable max-min value  $\mathcal{M}_{\varepsilon}$ ; (ii) a topological degree argument to obtain some estimate on  $\mathcal{M}_{\varepsilon}$ ; (iii) a compactness property of  $M_{\varepsilon}$  at the level  $\mathcal{M}_{\varepsilon}$ . After this we use a max-min theorem to obtain the existence of a saddle point of  $M_{\varepsilon}$  with critical value  $\mathcal{M}_{\varepsilon}$ . The upper bound on the number of peaks  $\ell \leq 6$  occurs in the proof of the compactness property; roughly speaking, we have to rule out some crucial configurations, like the *hexagon configuration* (i.e. a single point surrounded by other 6 points at the vertices of a regular hexagon), which cause a lack of *compactness* at the level  $\mathcal{M}_{\varepsilon}$ .

So we can conclude that our solutions are generated by the combination of three interactions effects which achieve an equilibrium for a suitable configuration of the peaks giving rise to the existence of multi-peak solutions. The interplay between each pair of peaks and also between each peak and the potential plays a crucial role.

The organization of the paper is the following. In Section 2 we derive the reduced problem; for the convenience of the reader we just state the main steps of the reduction process, postponing the details in Appendices A and B. In

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Section 3 we study the reduced problem and find a critical point of  $M_{\varepsilon}$  by a max-min procedure. Finally in Section 4 we study a geometrical problem where the crucial hexagon-configuration occurs.

Notation. Throughout the paper we will often use the notation C to denote generic positive constant.

The value of *C* is allowed to vary from place to place.

**Remark 1.2.** Combining assumptions (V3) and (f1) we deduce that a relationship between the possible degeneracy of  $P_0$  and the regularity of f is required. In particular Theorem 1.1 holds in the following two cases: m = 2 (i.e.  $P_0$  nondegenerate) and  $\sigma \ge \sqrt{2} - 1$  (i.e.  $p > \sqrt{2} + 1$  if  $f(t) = |t|^{p-2}t$ ), or  $m \ge 2$  generic and  $\sigma \ge \sqrt{3} - 1$  (i.e.  $p > \sqrt{3} + 1$  if  $f(t) = |t|^{p-2}t$ ). Moreover by assumption (V3) it follows that

$$\nabla V(P) \cdot \frac{P - P_0}{|P - P_0|} \ge C|P - P_0|^{l-1} \ge C\left(V(P) - V_0\right)^{\frac{l-1}{l}} \quad \text{as } P \to P_0$$

and

$$\left|\nabla V(P)\right| \leq C \left|P - P_0\right|^{l-1} \leq C \left(V(P) - V_0\right)^{\frac{l-1}{l}}$$
 as  $P \to P_0$ .

## 2. The reduction process: sketch of the proof

In this section we outline the main steps of the so called *finite-dimensional reduction*, which reduces the problem to finding a critical point for a functional on a finite dimensional space. We postpone the proofs and details to Appendices A and B.

Associated to (1.2) is the following energy functional:

$$J_{\varepsilon}: H^{1}_{V}(\Omega) \to \mathbb{R}, \quad J_{\varepsilon}[v] := \frac{1}{2} \int_{\Omega} \left( \varepsilon^{2} |\nabla v|^{2} + V(x)|v|^{2} \right) dx - \int_{\Omega} F(v) \, dx, \tag{2.7}$$

where  $F(t) = \int_0^t f(s) ds$  and

$$H_V^1(\Omega) = \left\{ v \in H_0^1(\Omega) \mid \int_{\Omega} V(x) |v|^2 \, dx < \infty \right\}$$

Let us equip  $H_V^1(\Omega)$  with the following scalar product:

$$(u,v)_{\varepsilon} = \int_{\Omega} \left( \varepsilon^2 \nabla u \nabla v + V(x) uv \right) dx.$$

It is well known that  $J_{\varepsilon} \in \mathscr{C}^2(H_V^1(\Omega), \mathbb{R})$  and the critical points of  $J_{\varepsilon}$  are the finite-energy solutions of (1.2). First we introduce the approximated solutions  $\chi w_{\mathbf{P}}$ . Let  $\Lambda$  be as in assumption (V2),  $\ell \ge 2$  and define the configuration space:

$$\Gamma_{\varepsilon} = \left\{ \mathbf{P} = (P_1, \dots, P_{\ell}) \in \Lambda^{N\ell} \mid V(P_i) - V_0 < \varepsilon^{2\beta} \; \forall i, \; w\left(\frac{P_i - P_j}{\varepsilon}\right) < \varepsilon^{2\beta} \; \text{for} \; i \neq j \right\},\$$

where  $\beta \in (\sigma, 1)$  is a number sufficiently close to 1.<sup>1</sup>

Observe that, according to (1.5),

$$\overline{\Gamma}_{\varepsilon} \subset \left\{ \mathbf{P} = (P_1, \dots, P_{\ell}) \in \Lambda^{N\ell} \mid V(P_i) - V_0 \leqslant \varepsilon^{2\beta} \; \forall i, \; |P_i - P_j| \geqslant \frac{2\beta^2}{\sqrt{V_0}} \varepsilon \log \frac{1}{\varepsilon} \text{ for } i \neq j \right\}.$$
(2.8)

For  $\mathbf{P} = (P_1, \ldots, P_\ell) \in \overline{\Gamma}_{\varepsilon}$  set

$$w_{P_i}(x) = w\left(\frac{x-P_i}{\varepsilon}\right), \qquad w_{\mathbf{P}} = \sum_{i=1}^{\ell} \lambda_i w_{P_i}, \quad \lambda_i \in \{-1, +1\}.$$

<sup>&</sup>lt;sup>1</sup> Observe that  $\Gamma_{\varepsilon}$  is nonempty, since for  $\varepsilon$  sufficiently small  $\{\mathbf{P} \mid |P_i - P_0| \le \varepsilon \log^2 \frac{1}{\varepsilon}, |P_i - P_j| \ge 2\beta \varepsilon \log \frac{1}{\varepsilon} \text{ for } i \ne j\} \subset \Gamma_{\varepsilon}$  thanks to assumption (V2) and (1.5).

Then consider  $\eta > 0$  sufficiently small such that  $\operatorname{dist}(\overline{\Lambda}, \partial \Omega) > \eta$  and let  $\chi \in \mathscr{C}_0^{\infty}(\Omega)$  be a cut-off function such that  $\chi(x) = 1$  if  $\operatorname{dist}(x, \Lambda) \leq \eta$ , so that it results  $\chi w_{P_i}, \chi w_{\mathbf{P}} \in H_V^1(\Omega)$ .

We look for a solution to (1.2) in a small neighbourhood of the first approximation  $\chi w_{\mathbf{P}}$ , i.e. solutions of the form as  $v := \chi w_{\mathbf{P}} + \phi$ , where the rest term  $\phi$  is *small*. To this aim we introduce the following functions:

$$Z_{P_i,n} = \left(V(x) - \varepsilon^2 \Delta\right) \frac{\partial(\chi w_{P_i})}{\partial x_n}, \quad i \in \{1, \dots, \ell\}, \ n \in \{1, \dots, N\}.$$

The object is to solve the following nonlinear problem: given  $\mathbf{P} = (P_1, \ldots, P_\ell) \in \overline{\Gamma}_{\varepsilon}$ , find  $(\phi, \alpha_{in})$  solving

$$\begin{cases} S_{\varepsilon}[\chi w_{\mathbf{P}} + \phi] = \sum_{i,n} \alpha_{in} Z_{P_{i},n}, \\ \phi \in H^{2}(\Omega) \cap H^{1}_{V}(\Omega), \quad \int_{\Omega} \phi Z_{P_{i},n} dx = 0, \quad i = 1, \dots, \ell, \ n = 1, \dots, N, \end{cases}$$

$$(2.9)$$

where

$$S_{\varepsilon}[v] = \varepsilon^2 \Delta v - V(x)v + f(v).$$
(2.10)

**Lemma 2.1.** Fix  $\tau = \beta^4(1 + \sigma)$ . Provided that  $\varepsilon > 0$  is sufficiently small, for every  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$  there is a pair  $(\phi_{\mathbf{P}}, \alpha_{in}(\mathbf{P})) \in (H^2(\Omega) \cap H^1_V(\Omega)) \times \mathbb{R}^{N\ell}$  satisfying (2.9) and

$$\|\phi_{\mathbf{P}}\|_{\infty} \leqslant \varepsilon^{\tau}, \quad (\phi_{\mathbf{P}}, \phi_{\mathbf{P}})_{\varepsilon} \leqslant C\varepsilon^{N+2\tau}, \quad \left|\alpha_{in}(\mathbf{P})\right| \leqslant \varepsilon^{1+\tau}.$$
(2.11)

Moreover the map  $\mathbf{P} \in \Gamma_{\varepsilon} \mapsto \phi_{\mathbf{P}} \in H^1_V(\Omega)$  is  $\mathscr{C}^1$ .

For  $\varepsilon > 0$  sufficiently small consider the reduced functional

$$M_{\varepsilon}:\overline{\Gamma}_{\varepsilon}\to\mathbb{R}, \quad M_{\varepsilon}[\mathbf{P}]:=\varepsilon^{-N}J_{\varepsilon}[\chi w_{\mathbf{P}}+\phi_{\mathbf{P}}]-c_{1}$$

where  $\phi_{\mathbf{P}}$  has been constructed in Lemma 2.1 and  $c_1 = \frac{\ell}{2} \int_{\mathbb{R}^N} |\nabla w|^2 dx - \ell \int_{\mathbb{R}^N} F(w) dx$ . Next proposition contains the key expansions of  $M_{\varepsilon}$  and  $\nabla M_{\varepsilon}$  (see Appendix B for the proof).

**Proposition 2.2.** The following expansion holds:

$$M_{\varepsilon}[\mathbf{P}] = c_2 \sum_{i=1}^{\ell} V(P_i) - c_3 \sum_{i \neq j} \lambda_i \lambda_j w \left(\frac{P_i - P_j}{\varepsilon}\right) + o(\varepsilon^{2\beta}), \qquad (2.12)$$

$$\nabla_{\mathbf{P}} M_{\varepsilon}[\mathbf{P}] = -c_3 \sum_{i \neq j} \lambda_i \lambda_j \nabla_{\mathbf{P}} \left( w \left( \frac{P_i - P_j}{\varepsilon} \right) \right) + o(\varepsilon^{2\beta - 1})$$
(2.13)

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ , where  $c_2, c_3 > 0$  are suitable constants.

According to Proposition 2.2 the potential term  $\sum_{i} V(P_i)$  becomes negligible with respect to the interaction term  $\sum_{i \neq j} \lambda_i \lambda_j w(\frac{P_i - P_j}{\varepsilon})$  in the computation of the gradient  $\nabla M_{\varepsilon}[\mathbf{P}]$ . However next proposition shows that there exists a direction where the contribution of the potential term prevails in the derivative of  $M_{\varepsilon}$  (see Appendix B for the proof).

**Proposition 2.3.** Let  $\mathbf{P}_k = (P_1^k, \dots, P_\ell^k) \in \Gamma_{\varepsilon_k}$  be a sequence such that

$$\liminf_{k\to\infty} \varepsilon_k^{-2\beta} \sum_{i=1}^{\ell} (V(P_i^k) - V_0) > 0.$$

Then, there exists a vector  $\mathbf{Q} = (Q_1, \dots, Q_\ell) \in \mathbb{R}^{N\ell}$  with  $|\mathbf{Q}| \leq \sqrt{\ell}$  such that, up to a subsequence

$$\nabla_{\mathbf{P}} M_{\varepsilon_k}[\mathbf{P}_k] \cdot \mathbf{Q} = c_2 (1 + o(1)) \sum_{i=1}^{\ell} \nabla V(P_i^k) \cdot Q_i \ge C \varepsilon_k^{2\beta \frac{l-1}{l}}$$
(2.14)

for some suitable C > 0, where  $c_2 > 0$  has been introduced in Proposition 2.2 and  $l \ge 2$  is given by assumption (V3). Furthermore

$$\nabla_{\mathbf{P}} \left[ w \left( \frac{P_i - P_j}{\varepsilon_k} \right) \right] \Big|_{\mathbf{P} = \mathbf{P}_k} \cdot \mathbf{Q} = \mathrm{o}(\varepsilon_k^2) \quad \text{for } i \neq j.$$

Finally next lemma concerns the relation between the critical points of  $M_{\varepsilon}$  and those of the energy functional  $J_{\varepsilon}$ .

**Lemma 2.4.** Let  $\mathbf{P}_{\varepsilon} \in \Gamma_{\varepsilon}$  be a critical point of  $M_{\varepsilon}$ . Then, provided that  $\varepsilon > 0$  is sufficiently small, the corresponding function  $v_{\varepsilon} = \chi w_{\mathbf{P}_{\varepsilon}} + \phi_{\mathbf{P}_{\varepsilon}}$  is a solution of (1.2).

#### 3. A max-min argument: proof of Theorem 1.1

According to Lemma 2.4 we just need to prove that the reduced functional  $M_{\varepsilon}$  has a critical point to find a solution of (1.2). Let  $h, h' \ge 1$  be such that

$$\ell := h + h' \leq 6 \quad \text{and} \quad (h, h') \neq (1, 5), (5, 1) \quad \text{if } N = 2.$$
(3.15)

In the following, for the sake of definiteness, we will assume  $h \leq h'$  and set

$$\lambda_i = (-1)^{i+1}$$
 if  $i = 1, ..., 2h$ ,  $\lambda_i = -1$  if  $i = 2h + 1, ..., \ell$ . (3.16)

We want to apply a max-min argument to characterize a topologically nontrivial critical value of  $M_{\varepsilon}$ . More precisely we are going to prove the existence of sets  $\mathscr{D}_{\varepsilon}$ , K,  $K_0 \subset \mathbb{R}^{N\ell}$  satisfying the following properties:

(P1)  $\mathscr{D}_{\varepsilon}$  is an open set with smooth boundary  $\partial \mathscr{D}_{\varepsilon}$ ,  $K_0$  and K are compact sets, K is connected and

$$K_0 \subset K \subset \mathscr{D}_{\varepsilon} \subset \mathscr{D}_{\varepsilon} \subset \Gamma_{\varepsilon}; \tag{3.17}$$

(P2) if we define the complete metric space  $\mathscr{F}$  by

$$\mathscr{F} = \{ \eta : K \to \mathscr{D}_{\varepsilon} \mid \eta \text{ continuous, } \eta(\mathbf{P}) = \mathbf{P} \ \forall \mathbf{P} \in K_0 \},\$$

then

$$\mathscr{M}_{\varepsilon} := \sup_{\eta \in \mathscr{F}} \min_{\mathbf{P} \in K} M_{\varepsilon} \big[ \eta(\mathbf{P}) \big] < \min_{\mathbf{P} \in K_0} M_{\varepsilon} [\mathbf{P}].$$
(3.18)

(P3) for every  $\mathbf{P} \in \partial \mathscr{D}_{\varepsilon}$  such that  $M_{\varepsilon}[\mathbf{P}] = \mathscr{M}_{\varepsilon}$ , there exists a vector  $\tau_{\mathbf{P}}$  tangent to  $\partial \mathscr{D}_{\varepsilon}$  at  $\mathbf{P}$  so that  $\partial_{\tau_{\mathbf{P}}} M_{\varepsilon}[\mathbf{P}] \neq 0$ .

Under these assumptions a critical point  $\mathbf{P}_{\varepsilon} \in \mathscr{D}_{\varepsilon}$  of  $M_{\varepsilon}$  with  $M_{\varepsilon}[\mathbf{P}_{\varepsilon}] = \mathscr{M}_{\varepsilon}$  exists, as a standard deformation argument involving the gradient flow of  $M_{\varepsilon}$  shows.

For the sake of simplicity we divide the proof into 4 steps.

The first step consists in the definition of a continuous map  $\mathbf{T}: \mathbb{R}^N \times (0, \infty)^{\ell-1} \to \mathbb{R}^{N\ell}$  with suitable properties which plays a key role in the crucial construction of the sets K,  $K_0$ : more precisely, K and  $K_0$  will be chosen in the range of  $\mathbf{T}$ .

Construction of a suitable map **T**. If  $\{\mathbf{e}_i\}$  denote the standard basis in  $\mathbb{R}^N$ , i.e.  $\mathbf{e}_i$  has the *j*th coordinate equal to 1 if j = i and equal to 0 if  $j \neq i$ , let us choose h' - h + 1 vectors (note that  $h' - h + 1 \leq 2N$  by (3.15))  $Z_1, Z_{2h+1}, \ldots, Z_\ell$  such that

$$\{Z_1, Z_{2h+1}, \ldots, Z_\ell\} \subset \{\pm \mathbf{e}_1, \pm \mathbf{e}_2, \ldots, \pm \mathbf{e}_N\}, \quad Z_i \neq Z_j \text{ for } i \neq j.$$

We construct a continuous function

$$\mathbf{T}: \mathbb{R}^N \times (0, \infty)^{\ell-1} \longrightarrow \mathbb{R}^{N\ell},$$
  
(P, **r**)  $\longmapsto \mathbf{T}_{P,\mathbf{r}} = (T_1(P, \mathbf{r}), \dots, T_\ell(P, \mathbf{r}))$ 

in the following way: for any  $P \in \mathbb{R}^N$  and  $\mathbf{r} = (r_2, \ldots, r_\ell) \in (0, \infty)^{\ell-1}$  set

$$\begin{cases} T_1(P, \mathbf{r}) = P, \\ T_i(P, \mathbf{r}) = P + \sum_{s=2}^{i} r_s Z_1 & \text{if } 2 \leq i \leq 2h, \\ T_i(P, \mathbf{r}) = P + r_i Z_i & \text{if } 2h + 1 \leq i \leq \ell. \end{cases}$$
(3.19)

We remark that it holds

$$|T_{j}(P,\mathbf{r}) - T_{i}(P,\mathbf{r})|^{2} \begin{cases} = (r_{i+1} + \dots + r_{j})^{2} & \text{if } 1 \leq i < j \leq 2h, \\ \ge (r_{2} + \dots + r_{i})^{2} + r_{j}^{2} & \text{if } 2 \leq i \leq 2h < j \leq \ell, \\ \ge r_{i}^{2} + r_{j}^{2} & \text{if } 2h + 1 \leq i < j \leq \ell \end{cases}$$
(3.20)

and

$$|T_i(P, \mathbf{r}) - P| = \begin{cases} 0 & \text{if } i = 1, \\ r_2 + \dots + r_i & \text{if } 2 \leqslant i \leqslant 2h, \\ r_i & \text{if } 2h + 1 \leqslant i \leqslant \ell. \end{cases}$$
(3.21)

By (3.20) and (3.21), recalling (3.16), we deduce that

$$r_{j} = \min_{i < j} |T_{j}(P, \mathbf{r}) - T_{i}(P, \mathbf{r})|, \quad j = 2, \dots, \ell,$$
(3.22)

$$\left|T_{i}(P,\mathbf{r}) - T_{j}(P,\mathbf{r})\right| \ge \sqrt{2} \min_{i=2,\dots,\ell} r_{i} \quad \text{if } \lambda_{i}\lambda_{j} = 1 \text{ and } i \neq j,$$
(3.23)

$$\left|T_{i}(P,\mathbf{r})-P\right| \leq 2h \max_{2 \leq i \leq \ell} r_{i}.$$
(3.24)

In the next step we are going to define the sets  $\mathscr{D}_{\varepsilon}$ , K,  $K_0$  for which properties (P1)–(P3) hold. As anticipated before, K will be defined as a subset of the range of the map **T**. To give an idea why this choice enables the max-min argument to work, let us make the following considerations. Thanks to (3.22) and (3.23) we have that  $\min_{\lambda_i = \lambda_j, i \neq j} |P_i - P_j| \ge \sqrt{2} \min_{\lambda_i = -\lambda_j} |P_i - P_j|$  if **P** lies in the range of **T**. Then, roughly speaking, using (1.5), the configurations in the range of **T** have the property that the interaction between the peaks of the same sign is negligible with respect to the interaction between opposite peaks. This implies  $\sum_{\lambda_i = \lambda_j, i \neq j} w(\frac{P_i - P_j}{\varepsilon}) = o(\varepsilon^{2\beta})$  for  $\mathbf{P} \in K$ . Let us analyze the other two terms which appear in  $M_{\varepsilon}$ : observe that  $\sum_{i=1}^{\ell} V(P_i)$  (which represents the potential effect) tends to cluster the points  $P_i$  at  $P_0$ , while the interaction term  $\sum_{\lambda_i = -\lambda_j} w(\frac{P_i - P_j}{\varepsilon})$  tends to repel the points  $P_i$  from each other. Then these two opposite effects give rise to a balance on K and such balance is quantitatively reflected in the max-min inequality (3.18).

Definition of the sets  $\mathscr{D}_{\varepsilon}$ , K,  $K_0$ . We define

$$\mathscr{D}_{\varepsilon} = \left\{ \mathbf{P} \in \Lambda^{N\ell} \mid c_2 \sum_{i=1}^{\ell} V(P_i) + c_3 \sum_{i \neq j} w \left( \frac{P_i - P_j}{\varepsilon} \right) < c_2 \ell V_0 + c_4 \varepsilon^{2\beta} \right\}$$

where  $c_4 = \min\{c_2, c_3\}$ . We immediately get  $\overline{\mathscr{D}}_{\varepsilon} \subset \Gamma_{\varepsilon}$ . Then let  $W_{\varepsilon}$  be the following open set of  $\mathbb{R}^{N+\ell-1}$ :

$$W_{\varepsilon} = \left\{ (P, \mathbf{r}) \mid \mathbf{T}_{P, \mathbf{r}} \in \Lambda^{N\ell}, \ c_2 \sum_{i=1}^{\ell} V(T_i(P, \mathbf{r})) + c_3 \sum_{i \neq j} w\left(\frac{T_i(P, \mathbf{r}) - T_j(P, \mathbf{r})}{\varepsilon}\right) < c_2 \ell V_0 + \frac{c_4}{2} \varepsilon^{2\beta} \right\}$$

where  $\mathbf{T}_{P,\mathbf{r}}$  is defined in (3.19).

Let us point that

$$(P_0, \mathbf{r}_{\varepsilon}) \in W_{\varepsilon}, \quad \text{where } \mathbf{r}_{\varepsilon} := (\rho_{\varepsilon}, \dots, \rho_{\varepsilon}) \in \mathbb{R}^{\ell-1} \quad \text{and} \quad \rho_{\varepsilon} = \frac{2\varepsilon}{\sqrt{V_0}} \log \frac{1}{\varepsilon}.$$
 (3.25)

Indeed according to (3.22),  $|T_i(P_0, \mathbf{r}_{\varepsilon}) - T_j(P_0, \mathbf{r}_{\varepsilon})| \ge \frac{2\varepsilon}{\sqrt{V_0}} \log \frac{1}{\varepsilon}$  for  $i \ne j$  and, by (1.5) we immediately check  $w(\frac{T_i(P_0, \mathbf{r}_{\varepsilon}) - T_j(P_0, \mathbf{r}_{\varepsilon})}{\varepsilon}) = o(\varepsilon^2)$  for  $i \ne j$ . Moreover, according to (3.24)  $|T_i(P_0, \mathbf{r}_{\varepsilon}) - P_0| \le \frac{4h\varepsilon}{\sqrt{V_0}} \log \frac{1}{\varepsilon}$  and by assumption (V2), we have  $V(T_i(P_0, \mathbf{r}_{\varepsilon})) = V_0 + O(\varepsilon^2 \log^2 \frac{1}{\varepsilon})$ .

Let  $U_{\varepsilon}$  be the connected component of  $W_{\varepsilon}$  containing  $(P_0, \mathbf{r}_{\varepsilon})$  and let us define

$$K = \{ \mathbf{T}_{P,\mathbf{r}} \in \mathbb{R}^{N\ell} \mid (P,\mathbf{r}) \in \overline{U}_{\varepsilon} \} \text{ and } K_0 = \{ \mathbf{T}_{P,\mathbf{r}} \in \mathbb{R}^{N\ell} \mid (P,\mathbf{r}) \in \partial U_{\varepsilon} \}.$$

*K* is connected and closed by construction since  $\overline{U}_{\varepsilon}$  is connected and closed. Furthermore it is obvious that  $K_0 \subset K \subset \mathscr{D}_{\varepsilon}$ .

Observe that according to assumption (V2) it results  $\sum_{i=1}^{\ell} V(P_i) > \ell V_0 + c$  for every  $\mathbf{P} \in \partial \Lambda^{N\ell}$  for some c > 0. Therefore  $K_0$  can be rewritten as

$$K_{0} = \left\{ \mathbf{T}_{P,\mathbf{r}} \mid (P,\mathbf{r}) \in \overline{U}_{\varepsilon}, \ c_{2} \sum_{i=1}^{\ell} V(T_{i}(P,\mathbf{r})) + c_{3} \sum_{i \neq j} w\left(\frac{T_{i}(P,\mathbf{r}) - T_{j}(P,\mathbf{r})}{\varepsilon}\right) = c_{2}\ell V_{0} + \frac{c_{4}}{2}\varepsilon^{2\beta} \right\}.$$
 (3.26)

It is useful to point out that

$$M_{\varepsilon}[\mathbf{T}_{P,\mathbf{r}}] = c_2 \sum_{i=1}^{\ell} V(T_i(P,\mathbf{r})) + c_3 \sum_{i \neq j} w\left(\frac{T_i(P,\mathbf{r}) - T_j(P,\mathbf{r})}{\varepsilon}\right) + o(\varepsilon^{2\beta}) \quad \text{unif. for } \mathbf{T}_{P,\mathbf{r}} \in K.$$
(3.27)

In fact, if  $\mathbf{T}_{P,\mathbf{r}} \in \overline{\Gamma}_{\varepsilon}$ , then by (2.8) and (3.22) we have  $r_i \ge \frac{2\beta^2}{\sqrt{V_0}} \varepsilon \log \frac{1}{\varepsilon}$ ; therefore, since  $2\sqrt{2\beta^2} > 2$  provided that  $\beta$  is sufficiently closed to 1, by (3.23) and (1.5) it follows

$$w\left(\frac{T_i(P,\mathbf{r}) - T_j(P,\mathbf{r})}{\varepsilon}\right) = o(\varepsilon^2) \quad \text{if } i \neq j \text{ and } \lambda_i \lambda_j = 1$$
(3.28)

uniformly for  $\mathbf{T}_{P,\mathbf{r}} \in K$ . By (3.28) and Proposition 2.2 estimate (3.27) follows.

We are going to prove the crucial inequality (3.18). We will use a topological degree argument. More precisely, the set *K* defined above is homeomorphic to the open connected set  $U_{\varepsilon} \subset \mathbb{R}^N \times (0, +\infty)^{\ell-1}$  and  $\partial U_{\varepsilon} \approx K_0$ . Therefore each continuous map  $\eta: K \to \mathscr{D}_{\varepsilon}$  such that  $\eta|_{K_0} = \text{id}$  induces a continuous map  $\tilde{\eta}: U_{\varepsilon} \to \mathbb{R}^N \times (0, +\infty)^{\ell-1}$  such that  $\tilde{\eta}|_{\partial U_{\varepsilon}} = \text{id}$ . Then we apply a topological degree argument to  $\tilde{\eta}$  to obtain an estimate on  $\min_{\mathbf{P} \in K} M_{\varepsilon}(\eta(\mathbf{P}))$  and, consequently, to compare  $\mathscr{M}_{\varepsilon}$  with  $\min_{\mathbf{P} \in K_0} M_{\varepsilon}(\mathbf{P})$ .

*Proof of (3.18).* Let  $\eta \in \mathscr{F}$ , namely  $\eta : K \to \mathscr{D}_{\varepsilon}$  is a continuous function such that  $\eta(\mathbf{P}) = \mathbf{P}$  for any  $\mathbf{P} \in K_0$ . Setting  $\eta = (\eta_1, \ldots, \eta_\ell)$  where  $\eta_i : K \to \mathbb{R}^N$ , let  $\tilde{\eta} : \overline{U}_{\varepsilon} \to \mathbb{R}^N \times \mathbb{R}^{\ell-1}$  be defined by

$$\tilde{\eta}_1(P, \mathbf{r}) = \eta_1(\mathbf{T}_{P, \mathbf{r}}) \text{ and } \tilde{\eta}_i(P, \mathbf{r}) = \min_{j < i} \left| \eta_i(\mathbf{T}_{P, \mathbf{r}}) - \eta_j(\mathbf{T}_{P, \mathbf{r}}) \right| \text{ for } i = 2, \dots, \ell.$$

First of all  $\tilde{\eta}$  is a continuous function, because of the continuity of  $\eta$ . Secondly, we claim that  $\tilde{\eta}(P, \mathbf{r}) = (P, \mathbf{r})$  for any  $(P, \mathbf{r}) \in \partial U_{\varepsilon}$ . In fact, if  $(P, \mathbf{r}) \in \partial U_{\varepsilon}$ , then by definition  $\mathbf{T}_{P,\mathbf{r}} \in K_0$ ; consequently  $\eta(\mathbf{T}_{P,\mathbf{r}}) = \mathbf{T}_{P,\mathbf{r}}$ , by which

$$\tilde{\eta}_1(\mathbf{T}_{P,\mathbf{r}}) = \eta_1(\mathbf{T}_{P,\mathbf{r}}) = T_1(P,\mathbf{r}) = P$$

while, using (3.22), for  $i \ge 2$ 

$$\tilde{\eta}_i(P, \mathbf{r}) = \min_{j < i} \left| \eta_i(\mathbf{T}_{P, \mathbf{r}}) - \eta_j(\mathbf{T}_{P, \mathbf{r}}) \right| = \min_{j < i} \left| T_i(P, \mathbf{r}) - T_j(P, \mathbf{r}) \right| = r_i$$

Hence the theory of the topological degree ensures that there exists  $(\overline{P}, \overline{\mathbf{r}}) \in U_{\varepsilon}$  such that  $\tilde{\eta}(\overline{P}, \overline{\mathbf{r}}) = (P_0, \mathbf{r}_{\varepsilon})$ , that is (see (3.25))

$$\eta_1(\mathbf{T}_{\overline{P},\mathbf{\tilde{r}}}) = P_0 \text{ and } \min_{j < i} \left| \eta_i(\mathbf{T}_{\overline{P},\mathbf{\tilde{r}}}) - \eta_j(\mathbf{T}_{\overline{P},\mathbf{\tilde{r}}}) \right| = \frac{2\varepsilon}{\sqrt{V_0}} \log \frac{1}{\varepsilon}, \quad i = 2, \dots, \ell.$$

In particular

$$\left|\eta_{i}(\mathbf{T}_{\overline{P},\mathbf{\tilde{r}}}) - \eta_{j}(\mathbf{T}_{\overline{P},\mathbf{\tilde{r}}})\right| \ge \frac{2\varepsilon}{\sqrt{V_{0}}}\log\frac{1}{\varepsilon} \quad \text{if } i \neq j$$

which implies

$$w\left(\frac{\eta_i(\mathbf{T}_{\overline{P},\bar{\mathbf{r}}}) - \eta_j(\mathbf{T}_{\overline{P},\bar{\mathbf{r}}})}{\varepsilon}\right) = o(\varepsilon^2) \quad \text{if } i \neq j.$$
(3.29)

Moreover, it is not difficult to check that

$$\left|\eta_{i}(\mathbf{T}_{\overline{P},\tilde{\mathbf{r}}}) - P_{0}\right| = \left|\eta_{i}(\mathbf{T}_{\overline{P},\tilde{\mathbf{r}}}) - \eta_{1}(\mathbf{T}_{\overline{P},\tilde{\mathbf{r}}})\right| \leq 2\ell \frac{\varepsilon}{\sqrt{V_{0}}} \log \frac{1}{\varepsilon}, \quad i = 2, \dots, \ell.$$

$$(3.30)$$

In fact, if i = 2 it holds  $|\eta_2(\mathbf{T}_{\overline{P}, \mathbf{\tilde{r}}}) - \eta_1(\mathbf{T}_{\overline{P}, \mathbf{\tilde{r}}})| = 2\frac{\varepsilon}{\sqrt{V_0}} \log \frac{1}{\varepsilon}$  and (3.30) follows. If i = 3 and  $|\eta_3(\mathbf{T}_{\overline{P}, \mathbf{\tilde{r}}}) - \eta_1(\mathbf{T}_{\overline{P}, \mathbf{\tilde{r}}})| = 2\frac{\varepsilon}{\sqrt{V_0}} \log \frac{1}{\varepsilon}$  then (3.30) follows. If  $|\eta_3(\mathbf{T}_{\overline{P}, \mathbf{\tilde{r}}}) - \eta_2(\mathbf{T}_{\overline{P}, \mathbf{\tilde{r}}})| = 2\frac{\varepsilon}{\sqrt{V_0}} \log \frac{1}{\varepsilon}$ , then

$$\left|\eta_{3}(\mathbf{T}_{\overline{P},\tilde{\mathbf{r}}}) - \eta_{1}(\mathbf{T}_{\overline{P},\tilde{\mathbf{r}}})\right| \leqslant \left|\eta_{3}(\mathbf{T}_{\overline{P},\tilde{\mathbf{r}}}) - \eta_{2}(\mathbf{T}_{\overline{P},\tilde{\mathbf{r}}})\right| + \left|\eta_{2}(\mathbf{T}_{\overline{P},\tilde{\mathbf{r}}}) - \eta_{1}(\mathbf{T}_{\overline{P},\tilde{\mathbf{r}}})\right| \leqslant 4\frac{\varepsilon}{\sqrt{V_{0}}}\log\frac{1}{\varepsilon}$$

and (3.30) follows. We iterate the procedure and we get estimate (3.30) for any index *i*.

By (3.30) and assumption (V2) it follows that

$$V\left(\eta_i(\mathbf{T}_{\overline{P},\overline{\mathbf{r}}})\right) = V_0 + O\left(\varepsilon^2 \log^2 \frac{1}{\varepsilon}\right).$$
(3.31)

Then by Proposition 2.2, (3.29) and (3.31), we deduce

$$\min_{\mathbf{T}_{P,\mathbf{r}}\in K} M_{\varepsilon} \big[ \eta(\mathbf{T}_{P,\mathbf{r}}) \big] \leqslant c_2 \ell V_0 + \mathrm{o} \big( \varepsilon^{2\beta} \big).$$

Hence

$$\mathscr{M}_{\varepsilon} = \sup_{\eta \in \mathscr{F}} \min_{\mathbf{T}_{P,\mathbf{r}} \in K} M_{\varepsilon} \Big[ \eta(\mathbf{T}_{P,\mathbf{r}}) \Big] \leqslant c_2 \ell V_0 + o(\varepsilon^{2\beta}).$$
(3.32)

On the other hand, by taking  $\eta(\mathbf{T}_{P,\mathbf{r}}) = \mathbf{T}_{P,\mathbf{r}}$  and using (3.27),

$$\mathscr{M}_{\varepsilon} \ge \min_{\mathbf{T}_{P,\mathbf{r}} \in K} \mathscr{M}_{\varepsilon}[\mathbf{T}_{P,\mathbf{r}}] \ge c_2 \ell V_0 + o(\varepsilon^{2\beta}).$$
(3.33)

Combining (3.32)–(3.33) we get

$$\mathscr{M}_{\varepsilon} = c_2 \ell V_0 + o(\varepsilon^{2\beta}). \tag{3.34}$$

On the other hand, combining (3.26) and (3.27)

$$\min_{\mathbf{T}_{P,\mathbf{r}}\in K_0} M_{\varepsilon}[\mathbf{T}_{P,\mathbf{r}}] = c_2\ell V_0 + \frac{c_4}{2}\varepsilon^{2\beta} + o(\varepsilon^{2\beta})$$

and (3.18) follows.

Once we have obtained a local linking geometrical structure, in order to apply a max-min argument to conclude the existence of a critical point we need to show a sort of compactness property for  $M_{\varepsilon}$ , more precisely we need to prove that the tangential component of the gradient of  $M_{\varepsilon}$  on  $\partial \mathscr{D}_{\varepsilon}$  is not zero at the level  $\mathscr{M}_{\varepsilon}$  (property (P3)). This is the aim of the last step of the proof, which is the most technical part. Let us outline the argument: since  $\partial \mathscr{D}_{\varepsilon}$  is defined as the level set of a  $\mathscr{C}^1$  function which consists of the same three main terms as  $M_{\varepsilon}$  and differs from  $M_{\varepsilon}$  only for the sign of one of these terms, according to the Lagrange theorem it is sufficient to rule out the existence of a critical point  $\mathbf{P} \in \partial \mathscr{D}_{\varepsilon}$  for the functional  $N_{\varepsilon}$  defined below such that  $M_{\varepsilon}(\mathbf{P}) = \mathscr{M}_{\varepsilon}$ . We will prove that for such  $\mathbf{P}$  two possibilities may occur: either  $\sum_{i=1}^{\ell} (V(P_i) - V_0) \ge C\varepsilon^{2\beta}$ , i.e. the potential term is *high*, and then Proposition 2.3 implies that the derivative of  $N_{\varepsilon}$  in a suitable direction is not zero, or  $V(P_i) - V_0 = o(\varepsilon^{2\beta})$  and  $w(\frac{P_i - P_j}{\varepsilon}) \ge C\varepsilon^{2\beta}$  for some  $i \neq j$ , i.e. one of the interaction between the peaks is *high*. In the latter case we expand the gradient of  $N_{\varepsilon}$  and analyze the leading term: we find out that its coefficient actually coincides with the gradient of a function  $\Phi : \mathbb{R}^{N\ell} \to \mathbb{R}$  for which a compactness property of the set of its critical points is proved if  $\ell \leq 6$  (see Lemma 4.2). For large numbers  $\ell \geq 6$  the method breaks down due to lack of compactness of the set of certain polygonal type configurations.

*Proof of (P3).* Observe that according to assumption (V2) it results  $\sum_{i=1}^{\ell} V(P_i) > \ell V_0 + c$  for every  $\mathbf{P} \in \partial \Lambda^{N\ell}$  for some c > 0; then

$$\partial \mathscr{D}_{\varepsilon} = \left\{ \mathbf{P} \in \Lambda^{N\ell} \mid c_2 \sum_{i=1}^{\ell} V(P_i) + c_3 \sum_{i \neq j} w \left( \frac{P_i - P_j}{\varepsilon} \right) = c_2 \ell V_0 + c_4 \varepsilon^{2\beta} \right\}.$$
(3.35)

It remains to prove that  $\partial \mathscr{D}_{\varepsilon}$  is smooth and that (P3) holds. According to the Lagrange theorem, assume by absurd that there exist sequences  $\varepsilon_k \to 0^+$ ,  $\mathbf{P}_k = (P_1^k, \dots, P_\ell^k) \in \partial \mathscr{D}_{\varepsilon_k}$ ,  $(\mu_{1,k}, \mu_{2,k}) \neq (0, 0)$  such that  $M_{\varepsilon_k}[\mathbf{P}_k] = \mathscr{M}_{\varepsilon_k}$  and  $\mathbf{P}_k$  is a critical point of the function

$$N_{\varepsilon_k}[\mathbf{P}] = \mu_{1,k} M_{\varepsilon_k}[\mathbf{P}] + \mu_{2,k} c_2 \sum_{i=1}^{\ell} V(P_i) + \mu_{2,k} c_3 \sum_{i \neq j} w \left(\frac{P_i - P_j}{\varepsilon_k}\right).$$

We will achieve the contradiction in three steps. *Step 1. Up to a subsequence*,

$$\sum_{i \neq j, \lambda_i \lambda_j = 1} w \left( \frac{P_i^k - P_j^k}{\varepsilon_k} \right) \ge C \varepsilon_k^{2\beta}.$$
(3.36)

Otherwise, it would be  $\sum_{i \neq j, \lambda_i \lambda_j = 1} w(\frac{P_i^k - P_j^k}{\varepsilon_k}) = o(\varepsilon_k^{2\beta})$  and consequently, by (3.35) and Proposition 2.2,

$$\mathscr{M}_{\varepsilon_k} = M_{\varepsilon_k}[\mathbf{P}_k] = c_2 \sum_{i=1}^{\ell} V(P_i^k) + c_3 \sum_{i \neq j} w\left(\frac{P_i^k - P_j^k}{\varepsilon_k}\right) + o(\varepsilon_k^{2\beta}) = c_2 \ell V_0 + c_4 \varepsilon_k^{2\beta} + o(\varepsilon_k^{2\beta}),$$

in contradiction with (3.34).

Step 2. There exists  $i_0 \neq j_0$  such that, up to a subsequence,

$$\frac{|\mu_{2,k}-\lambda_i\lambda_j\mu_{1,k}|}{|\mu_{1,k}|+|\mu_{2,k}|}w\bigg(\frac{P_{i_0}^k-P_{j_0}^k}{\varepsilon_k}\bigg)\geqslant C\varepsilon_k^{2\beta}.$$

If  $\mu_{2,k} = -(1 + o(1))\mu_{1,k}$ , then the thesis follows by (3.36).

Assume, up to a subsequence,  $\frac{|\mu_{2,k}+\mu_{1,k}|}{|\mu_{1,k}|+|\mu_{2,k}|} \ge C$ . Then we claim that  $\sum_{i=1}^{\ell} V(P_i^k) = \ell V_0 + o(\varepsilon_k^{2\beta})$ . Otherwise, by Proposition 2.3, there exists  $\mathbf{Q} = (Q_1, \dots, Q_\ell) \in \mathbb{R}^{N\ell}$  such that  $|\mathbf{Q}| \le \sqrt{\ell}$  and, up to a subsequence,

$$0 = \frac{1}{|\mu_{1,k}| + |\mu_{2,k}|} \left| \nabla_{\mathbf{P}} N_{\varepsilon_{k}}[\mathbf{P}_{k}] \cdot \mathbf{Q} \right| = c_{2} (1 + o(1)) \frac{|\mu_{1,k} + \mu_{2,k}|}{|\mu_{1,k}| + |\mu_{2,k}|} \left| \sum_{i=1}^{\ell} \nabla V(P_{i}^{k}) \cdot Q_{i} \right| + o(\varepsilon_{k}^{2}) \ge C \varepsilon_{k}^{2\beta^{\frac{l-1}{l}}}$$

and the contradiction follows. Consequently, by (3.35) and Proposition 2.2,

$$c_2\ell V_0 + o(\varepsilon_k^{2\beta}) = \mathscr{M}_{\varepsilon_k} = M_{\varepsilon_k}[\mathbf{P}_k] = c_2\ell V_0 + 2c_3 \sum_{i\neq j,\,\lambda_i\lambda_j=-1} w\left(\frac{P_i^k - P_j^k}{\varepsilon_k}\right) - c_4\varepsilon_k^{2\beta} + o(\varepsilon_k^{2\beta}),$$

which implies  $\sum_{i \neq j, \lambda_i \lambda_j = -1} w(\frac{P_i^k - P_j^k}{\varepsilon_k}) \ge C \varepsilon_k^{2\beta}$ , and then

$$\sum_{i\neq j,\,\lambda_i\lambda_j=-1}\frac{|\mu_{2,k}-\lambda_i\lambda_j\mu_{1,k}|}{|\mu_{1,k}|+|\mu_{2,k}|}w\bigg(\frac{P_i^k-P_j^k}{\varepsilon_k}\bigg)\geqslant C\varepsilon_k^{2\beta}.$$

Step 3. End of the proof. Up to a subsequence, we can split  $\{1, \ldots, \ell\} = I \cup J$  where

$$I = \left\{ i = 1, \dots, \ell \mid |P_i^k - P_{i_0}^k| \leq C\varepsilon_k \log \frac{1}{\varepsilon_k} \text{ for some } C > 0 \right\} \text{ and } J = \left\{ i = 1, \dots, \ell \mid \frac{|P_i^k - P_{i_0}^k|}{\varepsilon_k \log \frac{1}{\varepsilon_k}} \to \infty \right\}$$

Obviously  $i_0, j_0 \in I$ . Furthermore<sup>2</sup>

$$w\left(\frac{P_i^k - P_j^k}{\varepsilon_k}\right) = o(\varepsilon_k^2) \quad \forall i \in I, \ j \in J.$$

Up to a subsequence, we may assume

$$\sqrt{V_0} \frac{P_i^k - P_{i_0}^k}{2\beta\varepsilon_k \log \frac{1}{\varepsilon_k}} \to \overline{Q}_i \quad \forall i \in I$$

and

$$\varepsilon_k^{-2\beta} \frac{\mu_{2,k} - \lambda_i \lambda_j \mu_{1,k}}{|\mu_{1,k}| + |\mu_{2,k}|} w\left(\frac{P_i^k - P_j^k}{\varepsilon_k}\right) \to a_{ij} \quad \forall i, j \in I, \ i \neq j.$$

By Step 2 we immediately get  $a_{i_0j_0} \neq 0$ . Observe that, since  $w(\frac{P_i^k - P_j^k}{\varepsilon_k}) \leq \varepsilon_k^{2\beta}$  for  $i \neq j$ , by (1.5) we get  $|P_i^k - P_j^k| \geq (1 + o(1))2\frac{\beta}{\sqrt{V_0}}\varepsilon_k \log \frac{1}{\varepsilon_k}$ , by which

$$|\overline{Q}_i - \overline{Q}_j| \ge 1 \quad \forall i, j \in I, \ i \neq j.$$

$$(3.37)$$

Furthermore, if  $i, j \in I$  and  $a_{ij} \neq 0$ , then<sup>3</sup>  $|P_i^k - P_j^k| = 2\frac{\beta}{\sqrt{V_0}}(1 + o(1))\varepsilon_k \log \frac{1}{\varepsilon_k}$ , therefore,

$$|\overline{Q}_i - \overline{Q}_j| = 1 \quad \text{if } a_{ij} \neq 0, \ i, j \in I, \ i \neq j.$$
(3.38)

Finally, let us fix  $\bar{i} \in I$ ; by Proposition 2.2, since  $\nabla V(P_i^k) = O(\varepsilon_k^{2\beta \frac{l-1}{l}}) = o(\varepsilon_k^{2\beta - 1})$  by Remark 1.2, we compute

$$0 = \frac{1}{|\mu_{1,k}| + |\mu_{2,k}|} \frac{\partial}{\partial P_{\bar{i}}} \bigg|_{\mathbf{P}=\mathbf{P}_{k}} N_{\varepsilon_{k}}[\mathbf{P}_{k}] = c_{3} \sum_{i \neq j} \frac{\mu_{2,k} - \lambda_{i}\lambda_{j}\mu_{1,k}}{|\mu_{1,k}| + |\mu_{2,k}|} \frac{\partial}{\partial P_{\bar{i}}} \bigg|_{\mathbf{P}=\mathbf{P}_{k}} \left( w \left( \frac{P_{i} - P_{j}}{\varepsilon_{k}} \right) \right) + o(\varepsilon_{k}^{2\beta-1}) = 2c_{3} \sum_{j \neq \bar{i}, j \in I} \frac{\mu_{2,k} - \lambda_{\bar{i}}\lambda_{j}\mu_{1,k}}{|\mu_{1,k}| + |\mu_{2,k}|} \frac{1}{\varepsilon_{k}} w' \left( \frac{P_{\bar{i}}^{k} - P_{j}^{k}}{\varepsilon_{k}} \right) \frac{P_{\bar{i}}^{k} - P_{j}^{k}}{|P_{\bar{i}}^{k} - P_{j}^{k}|} + o(\varepsilon_{k}^{2\beta-1}).$$

By (1.5) we have  $w'(\frac{P_i^k - P_j^k}{\varepsilon_k}) = -(1 + o(1))w(\frac{P_i^k - P_j^k}{\varepsilon_k})$ ; therefore

$$0 = 2c_3\varepsilon_k^{2\beta-1} (1 + o(1)) \sum_{j \neq \overline{i}} a_{\overline{i}j} \frac{Q_{\overline{i}} - Q_j}{|\overline{Q}_{\overline{i}} - \overline{Q}_j|} + o(\varepsilon_k^{2\beta-1})$$

by which

$$\sum_{i\neq\bar{\imath},\,j\in I}a_{\bar{\imath}j}\frac{\overline{Q}_{\bar{\imath}}-\overline{Q}_{j}}{|\overline{Q}_{\bar{\imath}}-\overline{Q}_{j}|}=0$$

Therefore,  $\{\overline{Q}_i\}_{i \in I}$  is a critical point of the function

$$\sum_{i\neq j,\,i,\,j\in I}a_{ij}|Q_i-Q_j|$$

which satisfies (3.37) and (3.38). A contradiction arises because of Proposition 4.2.

**Proof of Theorem 1.1 completed.** According to Lemma 2.4, for  $\varepsilon > 0$  sufficiently small  $\chi w_{\mathbf{P}_{\varepsilon}} + \phi_{\mathbf{P}_{\varepsilon}}$  solves the problem (1.2), where  $\mathbf{P}_{\varepsilon} = (P_1^{\varepsilon}, \dots, P_{\ell}^{\varepsilon}) \in \Gamma_{\varepsilon}$  is the critical point of  $M_{\varepsilon}$  with critical value  $\mathscr{M}_{\varepsilon}$ . The construction of

<sup>2</sup> Indeed, if  $i \in I$  and  $j \in J$ , then  $\frac{P_i^k - P_j^k}{\varepsilon_k \log \frac{1}{\varepsilon_k}} \to \infty$ ; therefore, by (1.5),  $w(\frac{P_i^k - P_j^k}{\varepsilon_k}) = o(\varepsilon_k^m)$  for all m.

<sup>3</sup> Otherwise, up to a subsequence,  $|P_i^k - P_j^k| \ge 2\frac{\beta'}{\sqrt{V_0}}\varepsilon_k \log \frac{1}{\varepsilon_k}$  for some  $\beta' > \beta$ , by which, using (1.5),  $w(\frac{P_i^k - P_j^k}{\varepsilon_k}) = o(\varepsilon_k^{2\beta'})$ .

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the family  $\mathbf{P}_{\varepsilon}$  depends on the particular  $\beta \in (0, 1)$  chosen at the beginning of Section 3. To emphasize this fact we denote this family as  $\mathbf{P}_{\varepsilon,\beta}$ . Let  $\beta_k \subset (0, 1)$  be any sequence such that  $\beta_k \to 1$ . Then there is a decreasing sequence of positive numbers  $\varepsilon_k$  such that for all  $0 < \varepsilon < \varepsilon_k$  one has that  $\chi w_{\mathbf{P}_{\varepsilon,\beta_k}} + \phi_{\mathbf{P}_{\varepsilon,\beta_k}}$  solves (1.2),  $|P_i^{\varepsilon,\beta_k} - P_j^{\varepsilon,\beta_k}| \ge \frac{2\beta_k^{2\varepsilon}}{\sqrt{V_0}} \log \frac{1}{\varepsilon}$  for  $i \neq j$  and  $|\phi_{\mathbf{P}_{\varepsilon,\beta_k}}| \le \varepsilon^{\beta_k^4(1+\sigma)}$ . We define  $\mathbf{P}_{\varepsilon} = \mathbf{P}_{\varepsilon,\beta_k}$  and  $v_{\varepsilon} = \chi w_{\mathbf{P}_{\varepsilon,\beta_k}} + \phi_{\mathbf{P}_{\varepsilon,\beta_k}}$  if  $\varepsilon_{k+1} < \varepsilon < \varepsilon_k$  and we clearly have that the thesis of Theorem 1.1 holds.  $\Box$ 

#### 4. A configuration problem

**Lemma 4.1.** Let  $Q_1, \ldots, Q_\ell \in \mathbb{R}^N$  be  $\ell$  points satisfying the following

- (a)  $|Q_i Q_j| \ge 1$  for every  $i \ne j$ ;
- (b) setting  $\mathscr{A}_i = \{Q_i \mid |Q_i Q_j| = 1\}$ , then  $\#\mathscr{A}_i \ge 2$  for every *i*;
- (c) for every *i* the vectors  $\{Q_i Q_j\}_{Q_i \in \mathscr{A}_i}$  are linearly dependent.

Then it results:  $\ell \ge 6$  and  $\ell = 6$  if and only if  $Q_1, \ldots, Q_6$  lie on a 3-dimensional space and are located at the vertices of an octahedron with edge 1.

**Proof.** We distinguish the following cases.

1. There exists i such that  $\#\mathscr{A}_i = 2$ .

According to (c) there exist three aligned points at distance 1; up to a permutation of the indexes, we may assume that, denoting by  $\mathbf{e}_1$  the first vector of the standard basis of  $\mathbb{R}^N$ , i.e.  $\mathbf{e}_1 = (1, 0, \dots, 0)$ ,

$$Q_1 = \mathbf{e}_1, \qquad Q_2 = 2\mathbf{e}_1, \qquad \dots, \qquad Q_k = k\mathbf{e}_1, \qquad 0, (k+1)\mathbf{e}_1 \notin \{Q_1, \dots, Q_\ell\}$$
(4.39)

for some  $3 \le k \le \ell$ . By construction we have

$$\mathcal{A}_1 \cap \mathcal{A}_k = \{Q_2\} \quad \text{if } k = 3, \qquad \mathcal{A}_1 \cap \mathcal{A}_k = \emptyset \quad \text{if } k > 3,$$
  
$$\mathcal{A}_1 \cap \{Q_1, \dots, Q_k\} = \{Q_2\}, \qquad \mathcal{A}_k \cap \{Q_1, \dots, Q_k\} = \{Q_{k-1}\}.$$

Furthermore  $\#\mathscr{A}_1, \#\mathscr{A}_k \ge 3$ ; otherwise, if  $\#\mathscr{A}_1 = 2$ , then, since  $Q_2 \in \mathscr{A}_1$ , by (c) it would result  $\mathscr{A}_1 \subset \mathbb{R}\mathbf{e}_1$ , which is a contradiction with (4.39). So we conclude

$$\{Q_1,\ldots,Q_\ell\}\supset (\mathscr{A}_1\setminus\{Q_2\})\cup (\mathscr{A}_k\setminus\{Q_{k-1}\})\cup \{Q_1,Q_2,Q_k\}$$

with disjoint union, by which  $\ell \ge 2 + 2 + 3 = 7$ .

2. There exists a plane containing all the points  $Q_1, \ldots, Q_\ell$ .

Consider the convex hull of the set of points  $Q_1, \ldots, Q_\ell$ : up to a permutation of the indexes, we may assume that  $Q_1, \ldots, Q_k$ , with  $k \leq \ell$ , are the vertices of a polygon  $\mathscr{P}$  in a cyclic order with associated corners  $\theta_1, \ldots, \theta_k \in (0, \pi)$ . Then we have

$$\theta_1 + \dots + \theta_k = \pi (k-2).$$

Fix i = 1, ..., k. By (b) and (c) we get  $\# \mathscr{A}_i \ge 3$  and  $\mathscr{A}_i \subset \mathscr{P}$ ; therefore  $\theta_i \ge \frac{2}{3}\pi$ , by which

$$\pi(k-2) \geqslant k\frac{2}{3}\pi$$

and, consequently,  $k \ge 6$ . If  $k \ge 7$  the thesis follows. Assume k = 6; then  $\theta_i = \frac{2}{3}\pi$  for every i = 1, ..., k; hence the polygon  $\mathscr{P}$  is actually a regular hexagon with edge bigger or equal to 1: since we have  $|Q_1 - Q_i| > 1$  for  $i \ne 2, 6$ , then there exists j > 6 such that  $Q_j \in \mathscr{A}_1$ ; therefore  $\ell \ge 6 + 1 = 7$ .

*3. There exist i such that*  $\# \mathscr{A}_i = 3$ *.* 

Assume that i = 1 and  $\mathcal{A}_i = \mathcal{A}_1 = \{Q_2, Q_3, Q_4\}$ . According to (c) we have that  $Q_1, Q_2, Q_3, Q_4$  lie on a plane  $\alpha$ . Without loss of generality we may assume that  $\alpha = \{x_3 = \cdots = x_N = 0\}$ . Two of the points  $Q_2, Q_3, Q_4$  have distance at least  $\sqrt{3}$ , say  $|Q_3 - Q_4| \ge \sqrt{3}$ . Without loss of generality we may assume

$$Q_1 = 0,$$
  $Q_3 = (\cos \theta, \sin \theta, 0, ..., 0),$   $Q_4 = (\cos \theta, -\sin \theta, 0, ..., 0)$ 

with  $\frac{\pi}{3} \leq \theta \leq \frac{2}{3}\pi$ . We claim that

$$\mathscr{A}_3 \cap \mathscr{A}_4 \subset \{\mathcal{Q}_1, \mathcal{Q}_2\}. \tag{4.40}$$

Indeed let  $Q_j$  be such that  $|Q_j - Q_3| = |Q_j - Q_4| = 1$ . Then, setting  $Q_j = (x, y, \mathbf{z})$  with  $\mathbf{z} \in \mathbb{R}^{N-2}$ , we get

$$0 = |Q_j - Q_3|^2 - 1 = x^2 + y^2 + |\mathbf{z}|^2 - 2x\cos\theta - 2y\sin\theta = 0,$$
  

$$0 = |Q_j - Q_4|^2 - 1 = x^2 + y^2 + |\mathbf{z}|^2 - 2x\cos\theta + 2y\sin\theta = 0,$$

by which y = 0 and, consequently,

$$|Q_j|^2 = x^2 + y^2 + |\mathbf{z}|^2 = 2x\cos\theta.$$
(4.41)

In particular we get  $x^2 - 2x \cos \theta \le 0$ , that is  $|x| \le 2|\cos \theta|$ ; inserting this into (4.41) we deduce  $|Q_j|^2 \le 4\cos^2 \theta \le 1$ . Then either  $Q_i = 0 = Q_1$ , or  $|Q_i| = 1$ , that is  $Q_i \in \mathcal{A}_1$ , by which  $Q = Q_2$ . Hence we have proved (4.40).

Assume  $\#\mathscr{A}_3, \#\mathscr{A}_4 \ge 3$ . (Otherwise the thesis follows from step 1). If  $\#(\mathscr{A}_3 \setminus \{Q_1, Q_2\}) \ge 2$  or  $\#(\mathscr{A}_4 \setminus \{Q_1, Q_2\}) \ge 2$ , then

$$\{Q_1,\ldots,Q_\ell\}\supset\{Q_1,Q_2,Q_3,Q_4\}\cup\left(\mathscr{A}_3\setminus\{Q_1,Q_2\}\right)\cup\left(\mathscr{A}_4\setminus\{Q_1,Q_2\}\right)$$

with disjoint union, by which  $\ell \ge 4 + 3 = 7$ . Otherwise, assume  $\#(\mathscr{A}_3 \setminus \{Q_1, Q_2\}) = \#(\mathscr{A}_4 \setminus \{Q_1, Q_2\}) = 1$ , which implies  $\#\mathscr{A}_3 = \#\mathscr{A}_4 = 3$ . Then, according to (c), the points of  $\{Q_3, Q_j\}_{Q_j \in \mathscr{A}_3}$  lie on a plane; since  $Q_1, Q_2 \in \mathscr{A}_3$ , then  $\mathscr{A}_3 \subset \alpha$ . Analogously  $\mathscr{A}_4 \subset \alpha$ . Assume that there exists a point  $Q_j$  (j > 4) which does not lie on such plane (otherwise the thesis follows from case 2). Then

$$\{Q_1,\ldots,Q_\ell\}\supset\{Q_1,Q_2,Q_3,Q_4\}\cup\left(\mathscr{A}_3\setminus\{Q_1,Q_2\}\right)\cup\left(\mathscr{A}_4\setminus\{Q_1,Q_2\}\right)\cup\{j\}$$

with disjoint union, by which  $\ell \ge 4 + 1 + 1 + 1 = 7$ .

4.  $\# \mathscr{A}_i \ge 4$  for every *i*.

First observe that there exist at least two points such that  $|Q_i - Q_j| > 1$  (otherwise, according to (c), the points  $Q_1, \ldots, Q_\ell$  lie on a k-dimensional space with  $k \leq \ell - 2$ , then they cannot have mutual distance equal to 1.<sup>4</sup>) Then  $\ell \geq 6$ . Assume  $\ell = 6$  and  $|Q_1 - Q_6| > 1$  with

$$Q_1 = (0, \dots, 0, a), \qquad Q_6 = (0, \dots, 0, -a)$$

for some  $a > \frac{1}{2}$ . Then  $\mathscr{A}_1 = \mathscr{A}_6 = \{Q_2, Q_3, Q_4, Q_5\}$  and the points  $Q_2, Q_3, Q_4, Q_5$  lie on

$$\begin{cases} x_N = 0, \\ x_1^2 + x_2^2 + \dots + x_{N-1}^2 = \sqrt{1 - a^2}. \end{cases}$$

According to (c)  $Q_2$ ,  $Q_3$ ,  $Q_4$ ,  $Q_5$  lie on a two-dimensional subspace of  $\{x_N = 0\}$ , say  $\{x_3 = x_4 = \cdots = x_N = 0\}$ ; hence they are located on the circle

$$\begin{cases} x_3 = x_4 = \dots = x_N = 0, \\ x_1^2 + x_2^2 = \sqrt{1 - a^2}. \end{cases}$$

Then there exists a couple of the four points  $Q_2$ ,  $Q_3$ ,  $Q_4$ ,  $Q_5$  with mutual distance bigger than 1, say  $|Q_2 - Q_4| > 1$ , while, since  $\#\mathscr{A}_i \ge 4$  for every *i*, then  $|Q_2 - Q_3| = |Q_3 - Q_4| = |Q_4 - Q_5| = |Q_5 - Q_2| = 1$ . It follows that  $Q_2$ ,  $Q_3$ ,  $Q_4$ ,  $Q_5$  are the vertices of a square of edge 1; hence  $\sqrt{1 - a^2} = \frac{\sqrt{2}}{2}$ , i.e.  $a = \frac{\sqrt{2}}{2}$ .  $\Box$ 

**Lemma 4.2.** Let  $\ell \ge 2$  and consider the function

$$\Phi: (Q_1, \dots, Q_\ell) \in \mathbb{R}^{N\ell} \mapsto \sum_{\substack{i,j=1\\i\neq j}}^{\ell} a_{ij} |Q_i - Q_j|$$

where  $a_{ij} = a_{ji}$ . If  $\Phi$  is not identically zero and there exists  $(\overline{Q}_1, \ldots, \overline{Q}_\ell)$  a critical point of  $\Phi$  satisfying

 $|\overline{Q}_i - \overline{Q}_j| \ge 1 \quad \text{for } i \neq j \quad \text{and} \quad |\overline{Q}_i - \overline{Q}_j| = 1 \quad \text{if } a_{ij} \neq 0,$  (4.42)  $\text{then } \ell \ge 7.$ 

<sup>&</sup>lt;sup>4</sup> In general, in  $\mathbb{R}^k$  there are at most k + 1 points with mutual distance equal to 1.

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**Proof.** For every *i* set  $\mathscr{B}_i = \{\overline{Q}_j \mid a_{ij} \neq 0\}$ . First observe that we may assume without loss of generality  $\mathscr{B}_i \neq \emptyset$  for every *i*. Otherwise, assuming  $\{i \mid \exists j \neq i \text{ s.t. } a_{ij} \neq 0\} = \{1, \ldots, \ell'\}$  with  $1 \leq \ell' \leq \ell$ , we can replace  $\Phi$  by the new function  $(Q_1, \ldots, Q_{\ell'}) \in \mathbb{R}^{N\ell'} \mapsto \sum_{i,j \leq \ell', i \neq j} a_{ij} |Q_i - Q_j|$ .

It is easy to check that  $\#\mathscr{B}_i \ge 2$  for every  $i = 1, ..., \ell$ . Indeed, if  $\mathscr{B}_1 = \{\overline{Q}_2\}$  we get

$$0 = \partial_{Q_1} \Phi(\overline{Q}_1, \overline{Q}_2, \dots, \overline{Q}_\ell) = 2a_{12} \frac{\overline{Q}_1 - \overline{Q}_2}{|\overline{Q}_1 - \overline{Q}_2|}$$

in contradiction with (4.42).

Moreover it is also easy to prove that for every *i* the vectors  $\{\overline{Q}_i - \overline{Q}_j\}_{\overline{Q}_j \in \mathscr{B}_i}$  are linearly dependent. Indeed, for any *i* it holds

$$0 = \partial_{Q_i} \Phi(\overline{Q}_1, \overline{Q}_2, \dots, \overline{Q}_\ell) = 2 \sum_{\substack{j=1\\j\neq i}}^{\ell} a_{ij} \frac{\overline{Q}_i - \overline{Q}_j}{|\overline{Q}_i - \overline{Q}_j|}$$

and the claim follows.

Therefore, setting  $\mathscr{A}_i = \{\overline{Q}_j \mid |\overline{Q}_i - \overline{Q}_j| = 1\}$ , by (4.42) it follows that  $\mathscr{B}_i \subset \mathscr{A}_i$  and the points  $\overline{Q}_1, \ldots, \overline{Q}_\ell$  satisfy the assumption of Lemma 4.1, which implies  $\ell \ge 6$ .

Let us consider the case  $\ell = 6$ . According to Lemma 4.1, the points  $\overline{Q}_1, \ldots, \overline{Q}_6$  lie in a three-dimensional space and are located at the vertices of an octahedron of edge 1. Without loss of generality we assume

$$\overline{Q}_{1} := \frac{\sqrt{2}}{2} \mathbf{e}_{1} = \frac{\sqrt{2}}{2} (1, 0, 0, 0, \dots, 0), \qquad \overline{Q}_{2} := -\frac{\sqrt{2}}{2} \mathbf{e}_{1} = \frac{\sqrt{2}}{2} (-1, 0, 0, 0, \dots, 0),$$
  

$$\overline{Q}_{3} := \frac{\sqrt{2}}{2} \mathbf{e}_{2} = \frac{\sqrt{2}}{2} (0, 1, 0, 0, 0, \dots, 0), \qquad \overline{Q}_{4} := -\frac{\sqrt{2}}{2} \mathbf{e}_{2} = \frac{\sqrt{2}}{2} (0, -1, 0, 0, 0, \dots, 0),$$
  

$$\overline{Q}_{5} := \frac{\sqrt{2}}{2} \mathbf{e}_{3} = \frac{\sqrt{2}}{2} (0, 0, 1, 0, 0, \dots, 0), \qquad \overline{Q}_{6} := -\frac{\sqrt{2}}{2} \mathbf{e}_{3} = \frac{\sqrt{2}}{2} (0, 0 - 1, 0, 0, \dots, 0).$$

Since  $(\overline{Q}_1, \ldots, \overline{Q}_6)$  is a critical point of the function  $\Phi$ , we get that for any  $i = 1, \ldots, 6$  it holds

$$\sum_{\substack{j=1\\i\neq j}}^{6} a_{ij} \frac{\overline{Q}_i - \overline{Q}_j}{|\overline{Q}_i - \overline{Q}_j|} = 0.$$

Let us compute the previous expression when i = 1. We get  $a_{12} = 0$  since  $|\overline{Q}_1 - \overline{Q}_2| = \sqrt{2}$  and

$$\begin{cases} a_{13} + a_{14} + a_{15} + a_{16} = 0, \\ -a_{13} + a_{14} = 0, \\ -a_{15} + a_{16} = 0 \end{cases}$$

and so

$$a_{13} = a_{14} = -a_{15} = -a_{16}.$$

If we repeat the arguments above for any index *i* we easily get  $a_{12} = a_{34} = a_{56} = 0$  and

 $\left\{ \begin{array}{l} a_{13} = a_{14} = -a_{15} = -a_{16}, \\ a_{23} = a_{24} = -a_{25} = -a_{26}, \\ a_{13} = a_{23} = -a_{35} = -a_{36}, \\ a_{14} = a_{24} = -a_{45} = -a_{46}, \\ a_{15} = a_{25} = -a_{35} = -a_{45}, \\ a_{16} = a_{26} = -a_{36} = -a_{46} \end{array} \right.$ 

which implies  $a_{ij} = 0$  for any i, j = 1, ..., 6. That concludes the proof.  $\Box$ 

**Remark 4.3.** Observe that if  $\overline{Q}_1, \overline{Q}_2, \overline{Q}_3, \overline{Q}_4, \overline{Q}_5, \overline{Q}_6 \in \mathbb{R}^N$  are located at the vertices of a regular hexagon having edge 1 and centered at a seventh point  $\overline{Q}_7$ , then the set of points  $\{\overline{Q}_i\}_{1 \le i \le 7}$  satisfies (a)–(c) of Lemma 4.1.

**Remark 4.4.** Lemma 4.2 is optimal. Indeed set  $\lambda_7 = 1$  and  $\lambda_i = -1$  for i < 7. Then the *hexagon configuration*  $\{\overline{Q}_i\}_{1 \le i \le 7}$  of Remark 4.3 is critical for the function  $\sum_{i \ne j} a_{ij} |Q_i - Q_j|$  where

$$a_{ij} = \lambda_i \lambda_j$$
 if  $|\overline{Q}_i - \overline{Q}_j| = 1$  and  $a_{ij} = 0$  if  $|\overline{Q}_i - \overline{Q}_j| > 1$ .

#### Appendix A. Key energy estimate

Consider the configuration set  $\Gamma_{\varepsilon}$  and the approximated solutions  $\chi w_{\mathbf{P}}$  defined in Section 3. In this appendix we will derive some crucial estimates. We note that  $\chi w_{P_i} = w_{P_i}$  for  $|x - P_i| \leq \eta$ ; hence by (1.5) we deduce

$$|\chi w_{P_i} - w_{P_i}|, \ \varepsilon |\nabla(\chi w_{P_i}) - \nabla w_{P_i}|, \ \varepsilon^2 |D^2(\chi w_{P_i}) - D^2 w_{P_i}| = o(\varepsilon^4) w_{P_i}^{2/3}, \tag{A.43}$$

and, by assumption (f1),

$$F(\chi w_{\mathbf{P}}) - F(w_{\mathbf{P}}), \ f(\chi w_{\mathbf{P}}) - f(w_{\mathbf{P}}) = o(\varepsilon^4) \sum_{i=1}^{\ell} w_{P_i}^{2/3}, \qquad f'(\chi w_{\mathbf{P}}) - f'(w_{\mathbf{P}}) = o(\varepsilon^4) \sum_{i=1}^{\ell} w_{P_i}^{\sigma/2}$$
(A.44)

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ .

**Remark A.1.** By Remark 1.2 we have  $|\nabla V(P_i)| \leq C \varepsilon^{2\beta \frac{l-1}{l}} \leq C \varepsilon^{\beta}$  for  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$ ; then by (1.5) and assumption (V2) we deduce

$$\left|V(x)\chi w_{P_i} - V(P_i)w_{P_i}\right| \leq \left|\nabla V(P_i)\right| |x - P_i|w_{P_i} + C|x - P_i|^2 w_{P_i} \leq C\varepsilon^{1+\beta} w_{P_i}^{2/3},$$

by which

$$V(x)\chi w_{P_i} - V(P_i)w_{P_i} = O(\varepsilon^{1+\beta})w_{P_i}^{2/3}, \qquad V(x)\chi w_{P_i} - V_0w_{P_i} = O(\varepsilon^{2\beta})w_{P_i}^{2/3}$$
(A.45)

uniformly for  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$ .

Remark A.2. Observe that by (1.5) and (2.8) we immediately get

$$w_{P_i}(x)w_{P_j}(x) \leqslant Ce^{-\sqrt{V_0}\frac{|P_i - P_j|}{\varepsilon}} \leqslant C\varepsilon^{2\beta^2} \quad \text{for } i \neq j$$

uniformly for  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$ .

First we need the following result about the interaction of the  $w_{P_i}$ 's.

**Lemma A.3.** For  $i \neq j$  the following expansions hold

$$\int_{\mathbb{R}^{N}} f(w_{P_{i}})w_{P_{j}} dx = \varepsilon^{N} w \left(\frac{P_{i} - P_{j}}{\varepsilon}\right) \int_{\mathbb{R}^{N}} f(w) e^{\sqrt{V_{0}}x_{1}} dx + o(\varepsilon^{N+2\beta}),$$
$$\nabla_{\mathbf{P}} \left[ \int_{\mathbb{R}^{N}} f(w_{P_{i}})w_{P_{j}} dx \right] = \varepsilon^{N} \nabla_{\mathbf{P}} \left[ w \left(\frac{P_{i} - P_{j}}{\varepsilon}\right) \right] \int_{\mathbb{R}^{N}} f(w) e^{\sqrt{V_{0}}x_{1}} dx + o(\varepsilon^{N+2\beta-1})$$

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ .

Proof. The proof is an easy consequence of Lebesgue's Dominated Convergence Theorem. First consider the function

$$I(\rho) = \int_{\mathbb{R}^N} f(w)w(x+\rho \mathbf{e}_1) \, dx, \quad \rho > 0,$$

where  $\mathbf{e}_1$  is the first vector of the standard basis of  $\mathbb{R}^N$ , i.e.  $\mathbf{e}_1 = (1, 0, \dots, 0)$ . According to (1.5) for every  $x \in \mathbb{R}^N$  we have

$$\lim_{\rho \to \infty} \frac{w(x + \rho \mathbf{e}_1)}{w(\rho)} = \lim_{\rho \to \infty} e^{-\sqrt{V_0}|x + \rho \mathbf{e}_1| + \sqrt{V_0}\rho} = e^{-\sqrt{V_0}x_1}.$$
(A.46)

Furthermore

$$\frac{w(x+\rho\mathbf{e}_{1})}{w(\rho)} \leqslant C\left(\frac{\rho}{1+|x+\rho\mathbf{e}_{1}|}\right)^{\frac{N-1}{2}} e^{-\sqrt{V_{0}}|x+\rho\mathbf{e}_{1}|+\sqrt{V_{0}}\rho} \leqslant C\left(\frac{\rho}{1+|x+\rho\mathbf{e}_{1}|}\right)^{\frac{N-1}{2}} e^{\sqrt{V_{0}}|x|}.$$

Observe that  $\rho/(1 + |x + \rho \mathbf{e}_1|) \leq 2$  if  $|x| \leq \frac{\rho}{2}$ , while  $\rho/(1 + |x + \rho \mathbf{e}_1|) \leq 2|x|$  if  $|x| \geq \frac{\rho}{2}$ . Since, using assumption (f1),  $(2 + 2|x|)^{\frac{N-1}{2}} f(w) e^{\sqrt{V_0}|x|} \in L^1(\mathbb{R}^N)$ , then the convergence (A.46) is dominated. Hence we have proved that  $\frac{I(\rho)}{w(\rho)} \rightarrow \int_{\mathbb{R}^N} f(w) e^{\sqrt{V_0}x_1} dx$ . Next compute

$$I'(\rho) = \int_{\mathbb{R}^N} f(w)w'(x+\rho\mathbf{e}_1)\frac{x_1+\rho}{|x+\rho\mathbf{e}_1|}dx.$$

Using (1.5) and proceeding as above we get

$$\frac{I'(\rho)}{w'(\rho)} \to \int_{\mathbb{R}^N} f(w) e^{-\sqrt{V_0}x_1} dx.$$

Since

$$\int_{\mathbb{R}^N} f(w_{P_i}) w_{P_j} dx = \varepsilon^N \int_{\mathbb{R}^N} f(w) w \left( x + \frac{P_i - P_j}{\varepsilon} \right) dx = \varepsilon^N I \left( \frac{|P_i - P_j|}{\varepsilon} \right),$$

then the thesis follows.  $\Box$ 

Given  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$ , in the following we will make use of the following sets  $A_{\varepsilon,i}$  defined by

$$A_{\varepsilon,i} = \left\{ x \in \mathbb{R}^N \mid |x - P_i| \leqslant \frac{\beta^2}{\sqrt{V_0}} \varepsilon \log \frac{1}{\varepsilon} \right\}.$$
  
Observe that by (2.8)

$$A_{\varepsilon,i} \cap A_{\varepsilon,j} = \emptyset \quad \text{for } i \neq j \tag{A.47}$$

and, by using (1.5),

$$w_{P_i} \leqslant C \varepsilon^{\beta^2} \quad \text{on } \mathbb{R}^N \setminus A_{\varepsilon,i}.$$
 (A.48)

Next proposition provides an estimate of the error up to the functions  $\chi w_{\mathbf{P}}$  satisfies (1.2).

**Lemma A.4.** There exists a constant C > 0 such that for every  $\varepsilon > 0$  and  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$ :

$$\left|S_{\varepsilon}[\chi w_{\mathbf{P}}]\right| \leq C \varepsilon^{\beta^2(\beta^2+\sigma)} \sum_{i=1}^{\ell} w_{P_i}^{1-\beta^2}$$

where  $S_{\varepsilon}$  is the operator defined in (2.10).

**Proof.** By (A.43)–(A.45) we deduce

$$\varepsilon^{2} \Delta(\chi w_{\mathbf{P}}) - V(x)\chi w_{\mathbf{P}} + f(\chi w_{\mathbf{P}}) = \varepsilon^{2} \Delta w_{\mathbf{P}} - V_{0}w_{\mathbf{P}} + f(w_{\mathbf{P}}) + \mathcal{O}(\varepsilon^{2\beta}) \sum_{i=1}^{\ell} w_{P_{i}}^{2/3}$$
$$= f(w_{\mathbf{P}}) - \sum_{i=1}^{\ell} \lambda_{i} f(w_{P_{i}}) + \mathcal{O}(\varepsilon^{2\beta}) \sum_{i=1}^{\ell} w_{P_{i}}^{2/3}$$

uniformly for  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$ . Observe that by (A.47) it results  $\frac{|x-P_j|}{\varepsilon} \ge \frac{|x-P_j|}{\varepsilon}$  on  $A_{\varepsilon,i}$  for  $j \neq i$ ; since w is decreasing in |x|, we deduce  $w_{P_j} \le w_{P_i}$  on  $A_{\varepsilon,i}$  for  $j \neq i$ . Then, by using assumption (f1), we get

$$|f(w_{\mathbf{P}}) - \lambda_i f(w_{P_i})| \leq C w_{P_i}^{\sigma} \sum_{j \neq i} w_{P_j} \text{ on } A_{\varepsilon,i}.$$

(A.47)–(A.48) imply  $w_{P_j} \leq C \varepsilon^{\beta^2}$  on  $A_{\varepsilon,i}$  for  $j \neq i$ , by which, using also Remark A.2,

$$\left|f(w_{\mathbf{P}}) - \lambda_{i}f(w_{P_{i}})\right| \leqslant C\varepsilon^{\beta^{2}(\beta^{2}-\sigma)} \sum_{j\neq i} (w_{P_{i}}w_{P_{j}})^{\sigma} w_{P_{j}}^{1-\beta^{2}} \leqslant C\varepsilon^{\beta^{2}(\beta^{2}+\sigma)} \sum_{j\neq i} w_{j}^{1-\beta^{2}} \quad \text{on } A_{\varepsilon,i}.$$

On the other hand

$$|f(w_{P_i})| \leq C |w_{P_i}|^{1+\sigma} \leq C \varepsilon^{\beta^2(\beta^2+\sigma)} w_{P_i}^{1-\beta^2} \quad \text{on } \mathbb{R}^N \setminus A_{\varepsilon,i},$$
$$|f(w_{\mathbf{P}})| \leq C \sum_{i=1}^{\ell} |w_{P_i}|^{1+\sigma} \leq C \varepsilon^{\beta^2(\beta^2+\sigma)} \sum_{i=1}^{\ell} w_{P_i}^{1-\beta^2} \quad \text{on } \mathbb{R}^N \setminus \bigcup_{i=1}^{\ell} A_{\varepsilon,i}.$$

Since  $\beta^2(\beta^2 + \sigma) < 2\beta$  we obtain the thesis.  $\Box$ 

Lemma A.5. The following expansions hold

$$\int_{\substack{\mathbb{R}^N \setminus A_{\varepsilon,i} \\ \int \\ \mathbb{R}^N \setminus A_{\varepsilon,i}}} w_{P_i}^{2+\sigma} dx = o(\varepsilon^{N+2}),$$

$$\int_{\substack{\mathbb{R}^N \setminus A_{\varepsilon,i} \\ \int \\ A_{\varepsilon,i}}} w_{P_i}^{\sigma} w_{P_j} w_{P_k} dx = o(\varepsilon^{N+2}) \quad for \ j, k \neq i$$

uniformly for  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$ .

**Proof.** By (A.48) we have

 $w_{P_i}^{2+\sigma} \leqslant C \varepsilon^{2\beta^2 + rac{\sigma}{2}\beta^2} w_{P_i}^{rac{\sigma}{2}} \quad ext{on } \mathbb{R}^N \setminus A_{\varepsilon,i}.$ 

Combining Remark A.2 and (A.48) we get

$$w_{P_i}^{1+\sigma}w_{P_j} = (w_{P_i}w_{P_j})w_{P_i}^{\sigma} \leqslant C\varepsilon^{2\beta^2}w_{P_i}^{\sigma} \leqslant C\varepsilon^{2\beta^2+\frac{\sigma}{2}\beta^2}w_{P_i}^{\frac{\sigma}{2}} \quad \text{on } \mathbb{R}^N \setminus A_{\varepsilon,i} \text{ for } j \neq i.$$

(A.47)–(A.48) imply  $w_{P_j}, w_{P_k} \leq C \varepsilon^{\beta^2}$  on  $A_{\varepsilon,i}$  for  $j, k \neq i$ ; hence, using again Remark A.2,

$$w_{P_i}^{\sigma}w_{P_j}w_{P_k} = (w_{P_i}w_{P_j})^{\sigma}(w_{P_j}w_{P_k})^{1-\sigma}w_{P_k}^{\sigma} \leqslant C\varepsilon^{2\beta^2}w_{P_k}^{\sigma} \leqslant C\varepsilon^{2\beta^2+\frac{\sigma}{2}\beta^2}w_{P_k}^{\frac{\sigma}{2}} \quad \text{on } A_{\varepsilon,i} \text{ for } j, k \neq i.$$

If  $\beta$  is sufficiently close to 1, then it results  $2\beta^2 + \frac{\sigma}{2}\beta^2 > 2$ ; therefore, after integration, we obtain the thesis.  $\Box$ 

With the help of Lemmas A.3 and A.5 we derive the following key energy estimate.

Proposition A.6. The following asymptotic expansions hold:

$$J_{\varepsilon}[\chi w_{\mathbf{P}}] = c_{1}\varepsilon^{N} + c_{2}\varepsilon^{N}\sum_{i=1}^{\varepsilon}V(P_{i}) - c_{3}\varepsilon^{N}\sum_{i\neq j}\lambda_{i}\lambda_{j}w\left(\frac{P_{i}-P_{j}}{\varepsilon}\right) + o(\varepsilon^{N+2\beta}),$$
  

$$\nabla_{\mathbf{P}}(J_{\varepsilon}[\chi w_{\mathbf{P}}]) = -c_{3}\varepsilon^{N}\sum_{i\neq j}\lambda_{i}\lambda_{j}\nabla_{\mathbf{P}}\left(w\left(\frac{P_{i}-P_{j}}{\varepsilon}\right)\right) + o(\varepsilon^{N+2\beta-1})$$
(A.49)

uniformly for  $\mathbf{P} = (P_1, \ldots, P_\ell) \in \Gamma_{\varepsilon}$ , where the constants  $c_1, c_2, c_3$  are given by

$$c_{1} = \frac{\ell}{2} \int_{\mathbb{R}^{N}} |\nabla w|^{2} dx - \ell \int_{\mathbb{R}^{N}} F(w) dx, \qquad c_{2} = \frac{1}{2} \int_{\mathbb{R}^{N}} w^{2}, \qquad c_{3} = \frac{1}{2} \int_{\mathbb{R}^{N}} f(w) e^{\sqrt{V_{0}x_{1}}} dx.$$

**Proof.** We begin by estimating the potential term: by (A.43) and (A.45) we derive

$$\int_{\Omega} V(x) |w_{\mathbf{P}}|^2 dx = \sum_{i=1}^{\ell} \int_{\Omega} V(x) |\chi w_{P_i}|^2 dx + \sum_{i \neq j} \lambda_i \lambda_j \int_{\Omega} V(x) \chi w_{P_i} \chi w_{P_j} dx$$
$$= \sum_{i=1}^{\ell} V(P_i) \varepsilon^N \int_{\mathbb{R}^N} w^2 dx + \sum_{i \neq j} \lambda_i \lambda_j V(P_i) \int_{\mathbb{R}^N} w_{P_i} w_{P_j} dx + o(\varepsilon^{N+2\beta})$$
(A.50)

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ . Remark A.2 implies

$$\left(V(P_i) - V_0\right) \int_{\mathbb{R}^N} w_{P_i} w_{P_j} dx = o\left(\varepsilon^{N+2\beta}\right)$$
(A.51)

for  $i \neq j$  and, by (A.43) and (A.44) it follows

$$\frac{\varepsilon^{2}}{2} \int_{\Omega} |\nabla(\chi w_{\mathbf{P}})|^{2} dx - \int_{\Omega} F(\chi w_{\mathbf{P}}) dx = \frac{\varepsilon^{2}}{2} \int_{\mathbb{R}^{N}} |\nabla w_{\mathbf{P}}|^{2} dx - \int_{\Omega} F(w_{\mathbf{P}}) dx + o(\varepsilon^{N+2})$$

$$= \ell \frac{\varepsilon^{N}}{2} \int_{\mathbb{R}^{N}} |\nabla w|^{2} dx - \ell \varepsilon^{N} \int_{\mathbb{R}^{N}} F(w) dx + \frac{\varepsilon^{2}}{2} \sum_{i \neq j} \lambda_{i} \lambda_{j} \int_{\mathbb{R}^{N}} \nabla w_{P_{i}} \nabla w_{P_{j}} dx$$

$$- \int_{\mathbb{R}^{N}} \left( F(w_{\mathbf{P}}) - \sum_{i=1}^{\ell} F(w_{P_{i}}) \right) dx + o(\varepsilon^{N+2})$$
(A.52)

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ . Combining (A.50)–(A.52), and using (1.3), we get

$$J_{\varepsilon}[\chi w_{\mathbf{P}}] = c_{1}\varepsilon^{N} + c_{2}\varepsilon^{N} \sum_{i=1}^{\ell} V(P_{i}) + \frac{1}{2} \sum_{i \neq j} \lambda_{i}\lambda_{j} \int_{\mathbb{R}^{N}} f(w_{P_{i}})w_{P_{j}} dx$$
$$- \int_{\mathbb{R}^{N}} \left( F(w_{\mathbf{P}}) - \sum_{i=1}^{\ell} F(w_{P_{i}}) \right) dx + o\left(\varepsilon^{N+2\beta}\right)$$
$$= c_{1}\varepsilon^{N} + c_{2}\varepsilon^{N} \sum_{i=1}^{\ell} V(P_{i}) - \frac{1}{2} \sum_{i \neq j} \lambda_{i}\lambda_{j} \int_{\mathbb{R}^{N}} f(w_{P_{i}})w_{P_{j}} dx - H(\mathbf{P}) + o\left(\varepsilon^{N+2\beta}\right), \tag{A.53}$$

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ , where we have set

$$H(\mathbf{P}) = \int_{\mathbb{R}^N} F(w_{\mathbf{P}}) \, dx - \sum_{i=1}^{\ell} \int_{\mathbb{R}^N} F(w_{P_i}) \, dx - \sum_{i \neq j} \lambda_i \lambda_j \int_{\mathbb{R}^N} f(w_{P_i}) w_{P_j} \, dx, \quad \mathbf{P} \in \overline{\Gamma}_{\varepsilon}.$$

Consider the sets  $A_{\varepsilon,i}$  defined in Lemma A.5; we can write  $H(\mathbf{P}) = H_1(\mathbf{P}) + H_2(\mathbf{P})$ , where

$$H_1(\mathbf{P}) = \sum_{i=1}^{\ell} \int_{A_{\varepsilon,i}} \left( F(w_{\mathbf{P}}) - F(w_{P_i}) - f(w_{P_i}) \sum_{j \neq i} \lambda_i \lambda_j w_{P_j} \right) dx,$$

and, using assumption (f1),

$$|H_2(\mathbf{P})| \leq C \sum_{i=1}^{\ell} \int_{\mathbb{R}^N \setminus A_{\varepsilon,i}} \left( w_{P_i}^{2+\sigma} + w_{P_i}^{1+\sigma} \sum_{j \neq i} w_{P_j} \right) dx.$$

Observe that  $\frac{|x-P_j|}{\varepsilon} \ge \frac{|x-P_i|}{\varepsilon}$  on  $A_{\varepsilon,i}$  for  $j \neq i$ , by which, since w is decreasing in |x|,  $w_{P_j} \le w_{P_i}$  on  $A_{\varepsilon,i}$ . Then, by using assumption (f1), we get

$$\left|F(w_{\mathbf{P}}) - F(w_{P_i}) - f(w_{P_i})\sum_{j\neq i}\lambda_i\lambda_j w_{P_j}\right| \leqslant C w_{P_i}^{\sigma} \sum_{j\neq i} w_{P_j}^2 \quad \text{on } A_{\varepsilon,i}.$$

By applying Lemma A.5 we achieve  $H(\mathbf{P}) = o(\varepsilon^{N+2})$ . Then by (A.53), using Lemma A.3, we obtain (A.49). We are going to estimate the error term  $o(\varepsilon^{N+2\beta})$  in (A.49) in the  $\mathscr{C}^1$  sense. To this aim, fix  $i \in \{1, \dots, \ell\}$  and  $n \in \{1, \dots, N\}$ ; denoting by  $P_i^n$  the *n*th component of  $P_i$ , by definition we have  $\frac{\partial w_P}{\partial P_i^n} = -\lambda_i \frac{\partial w_{P_i}}{\partial x_n}$ . Then we can compute

$$\lambda_{i} \frac{\partial J_{\varepsilon}[\chi w_{\mathbf{P}}]}{\partial P_{i}^{n}} = -\left\langle J_{\varepsilon}'[\chi w_{\mathbf{P}}], \chi \frac{\partial w_{P_{i}}}{\partial x_{n}} \right\rangle = \int_{\Omega} \left( \varepsilon^{2} \Delta(\chi w_{\mathbf{P}}) - V(x) \chi w_{\mathbf{P}} + f(\chi w_{\mathbf{P}}) \right) \chi \frac{\partial w_{P_{i}}}{\partial x_{n}} dx$$
$$= \int_{\mathbb{R}^{N}} \left( \varepsilon^{2} \sum_{j=1}^{\ell} \lambda_{j} \Delta w_{P_{j}} - \sum_{j=1}^{\ell} \lambda_{j} V(P_{j}) w_{P_{j}} + f(w_{\mathbf{P}}) \right) \frac{\partial w_{P_{i}}}{\partial x_{n}} dx + O(\varepsilon^{N+\beta})$$

by (A.43), (A.44) and (A.45). By Remark A.2 it follows that for  $j \neq i$ 

$$\left(V(P_j) - V_0\right) \int_{\mathbb{R}^N} w_{P_j} \left| \frac{\partial w_{P_i}}{\partial x_n} \right| dx \leqslant C \varepsilon^{-1} \left(V(P_j) - V_0\right) \int_{\mathbb{R}^N} w_{P_j} w_{P_i} dx \leqslant C \varepsilon^{N+\beta}$$

(provided that  $\beta$  is sufficiently closed to 1), while  $\int_{\mathbb{R}^N} w_{P_i} \frac{\partial w_{P_i}}{\partial x_n} dx = \frac{1}{2} \int_{\mathbb{R}^N} \frac{\partial w_{P_i}^2}{\partial x_n} dx = 0$ . Then, using (1.3) we arrive at

$$\lambda_{i} \frac{\partial J_{\varepsilon}[\chi w_{\mathbf{P}}]}{\partial P_{i}^{n}} = \int_{\mathbb{R}^{N}} \left( \varepsilon^{2} \sum_{j=1}^{\ell} \lambda_{j} \Delta w_{P_{j}} - V_{0} \sum_{j=1}^{\ell} \lambda_{j} w_{P_{j}} + f(w_{\mathbf{P}}) \right) \frac{\partial w_{P_{i}}}{\partial x_{n}} dx + O(\varepsilon^{N+\beta})$$
$$= \int_{\mathbb{R}^{N}} \left( f(w_{\mathbf{P}}) - \sum_{j=1}^{\ell} \lambda_{j} f(w_{P_{j}}) \right) \frac{\partial w_{P_{i}}}{\partial x_{n}} dx + O(\varepsilon^{N+\beta})$$
$$= \sum_{j \neq i} \lambda_{j} \int_{\mathbb{R}^{N}} f'(w_{P_{i}}) w_{P_{j}} \frac{\partial w_{P_{i}}}{\partial x_{n}} dx + K_{1}(\mathbf{P}) + K_{2}(\mathbf{P}) + K_{3}(\mathbf{P}) + O(\varepsilon^{N+\beta})$$

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ , where

$$K_{1}(\mathbf{P}) = \int_{A_{\varepsilon,i}} \left( f(w_{\mathbf{P}}) - \lambda_{i} f(w_{P_{i}}) - f'(w_{P_{i}}) \sum_{j \neq i} \lambda_{j} w_{P_{j}} \right) \frac{\partial w_{P_{i}}}{\partial x_{n}} dx,$$
  

$$K_{2}(\mathbf{P}) = \sum_{j \neq i} \int_{A_{\varepsilon,j}} \left( f(w_{\mathbf{P}}) - \lambda_{j} f(w_{P_{j}}) \right) \frac{\partial w_{P_{i}}}{\partial x_{n}} dx$$

and, using assumption (f1),

$$\left|K_{3}(\mathbf{P})\right| \leqslant C \sum_{j=1}^{\ell} \int_{\mathbb{R}^{N} \setminus A_{\varepsilon,j}} w_{P_{j}}^{1+\sigma} \left|\frac{\partial w_{P_{i}}}{\partial x_{n}}\right| + \sum_{j \neq i} \int_{\mathbb{R}^{N} \setminus A_{\varepsilon,i}} w_{P_{i}}^{\sigma} w_{P_{j}} \left|\frac{\partial w_{P_{i}}}{\partial x_{n}}\right| dx.$$

Since  $|\frac{\partial w_{P_i}}{\partial x_n}| \leq C\varepsilon^{-1}w_{P_i}$  according to (1.5), by Lemma A.5 we immediately get  $|K_3(\mathbf{P})| = o(\varepsilon^{N+1})$  uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ . By assumption (f1) we get

$$\left|f(w_{\mathbf{P}})-\lambda_{i}f(w_{P_{i}})-f'(w_{P_{i}})\sum_{j\neq i}\lambda_{j}w_{P_{j}}\right|\leqslant C\sum_{j\neq i}w_{P_{j}}^{1+\sigma}.$$

Using Lemma A.5 we deduce  $K_1(\mathbf{P}) = o(\varepsilon^{N+1})$  uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ . Finally fix  $j \neq i$ : since  $w_{P_k} \leq w_{P_j}$  on  $A_{\varepsilon,j}$  for  $k \neq j$ , we have

$$\left|f(w_{\mathbf{P}}) - \lambda_{j}f(w_{P_{j}})\right| \left|\frac{\partial w_{P_{i}}}{\partial x_{n}}\right| \leq C\varepsilon^{-1}w_{P_{j}}^{\sigma}w_{P_{i}}\sum_{k\neq j}w_{P_{k}} \text{ on } A_{\varepsilon,j}.$$

Integrating over  $A_{\varepsilon, j}$  and using Lemma A.5,  $K_2(\mathbf{P}) = o(\varepsilon^{N+1})$  uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ . Thus we have obtained

$$\frac{\partial J_{\varepsilon}[\chi w_{\mathbf{P}}]}{\partial P_{i}^{n}} = \sum_{j \neq i} \lambda_{i} \lambda_{j} \int_{\mathbb{R}^{N}} f'(w_{P_{i}}) w_{P_{j}} \frac{\partial w_{P_{i}}}{\partial x_{n}} dx + O(\varepsilon^{N+\beta}) = -\frac{\partial}{\partial P_{i}^{n}} \sum_{j \neq i} \lambda_{i} \lambda_{j} \int_{\mathbb{R}^{N}} f(w_{P_{i}}) w_{P_{j}} dx + O(\varepsilon^{N+\beta})$$

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ , and the second part of the thesis follows by using Lemma A.3.  $\Box$ 

## Appendix B. Lyapunov–Schmidt reduction

In this appendix we carry out the reduction procedure which was sketched in Section 3. In particular we will prove Lemma 2.1, Proposition 2.2 and Lemma 2.4. A large part of the proofs follows in a standard way but we include some details here for completeness.

### B.1. The linearized equation

Consider the functions  $Z_{P_i,n}$  defined in Section 3. Observe that by proceeding as in Remark A.1 we deduce

$$\left|V(x) - V(P_i)\right| \left|\frac{\partial(\chi w_{P_i})}{\partial x_n}\right| \leq C \varepsilon^{\beta} w_{P_i}^{2/3}$$

by which, using (A.43), we get

$$Z_{P_i,n} = \left(V_0 - \varepsilon^2 \Delta\right) \frac{\partial w_{P_i}}{\partial x_n} + \mathcal{O}\left(\varepsilon^{2\beta - 1}\right) w_{P_i}^{2/3} = f'(w_{P_i}) \frac{\partial w_{P_i}}{\partial x_n} + \mathcal{O}\left(\varepsilon^{2\beta - 1}\right) w_{P_i}^{2/3}$$
(B.54)

uniformly for  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$ . After integration by parts it is immediate to prove that

$$\left(\phi, \frac{\partial(\chi w_{P_i})}{\partial x_n}\right)_{\varepsilon} = \int_{\Omega} \phi Z_{P_i, n} \, dx \quad \forall \phi \in H^1_V(\Omega), \tag{B.55}$$

then orthogonality to the functions  $\frac{\partial(\chi w_{P_i})}{\partial x_n}$  in  $H_V^1(\Omega)$  with respect to the scalar product  $(\cdot, \cdot)_{\varepsilon}$  is equivalent to orthogonality to  $Z_{P_i,n}$  in  $L^2(\Omega)$ . Hence we easily get

$$\int_{\Omega} Z_{P_i,n} \frac{\partial(\chi w_{P_j})}{\partial x_m} dx = \delta_{ij} \delta_{nm} \varepsilon^{N-2} \left\| \frac{\partial w}{\partial x_1} \right\|_{H^1(\mathbb{R}^N)}^2 + o(\varepsilon^{N-2})$$
(B.56)

uniformly for  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$  ( $\delta_{ij}$  and  $\delta_{nm}$  denoting the Kronecker's symbols), where  $\|v\|_{H^1(\mathbb{R}^N)}^2 := \int_{\mathbb{R}^N} (|\nabla v|^2 + V_0 |v|^2) dx$ . Let  $\mu \in (0, \sigma)$  be a sufficiently small number and introduce the following weighted norm:

$$\|\phi\|_{\star,\mathbf{P}} := \sup_{x \in \Omega} \sum_{i=1}^{\ell} w_{P_i}^{-\mu}(x) |\phi(x)|,$$
(B.57)

and the spaces

$$C_{\star,\mathbf{P}} = \left\{ \phi \in \mathscr{C}(\overline{\Omega}) \mid \|\phi\|_{\star,\mathbf{P}} < \infty \right\}, \qquad H^2_{\star,\mathbf{P}} = H^2(\Omega) \cap C_{\star,\mathbf{P}}.$$

We first consider a linear problem: taken  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$  and given  $\theta \in C_{*,\mathbf{P}}$ , find a function  $\phi$  and constants  $\alpha_{in}$  satisfying

$$\begin{cases}
L_{\mathbf{P}}[\phi] = \theta + \sum_{i,n} \alpha_{in} Z_{P_{i,n}}, \\
\phi \in H^{2}_{\star,\mathbf{P}}(\Omega) \cap H^{1}_{V}(\Omega), \quad \int_{\Omega} \phi Z_{P_{i,n}} dx = 0 \quad \text{for } i = 1, \dots, \ell, \ n = 1, \dots, N,
\end{cases}$$
(B.58)

where

$$L_{\mathbf{P}}[\phi] := \varepsilon^2 \Delta \phi - V(x)\phi + f'(\chi w_{\mathbf{P}})\phi$$

**Lemma B.1.** There exists a constant C > 0 such that, provided that  $\varepsilon$  is sufficiently small, if  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$  and  $(\phi, \theta, \alpha_{in})$  satisfies (B.58), then

$$|\alpha_{in}| \leqslant C((\varepsilon^{2\beta^2\sigma+1}+\varepsilon^{2\beta})\|\phi\|_{*,\mathbf{P}}+\varepsilon\|\theta\|_{*,\mathbf{P}}).$$

**Proof.** Consider  $\varepsilon_k \to 0$  a generic sequence and  $\mathbf{P}_k = (P_1^k, \dots, P_\ell^k) \in \overline{\Gamma}_{\varepsilon_k}$ ,  $(\phi_k, \theta_k, \alpha_{in}^k)$  satisfying (B.58). Let  $(j, m) \in \{1, \dots, \ell\} \times \{1, \dots, N\}$  be such that, up to a subsequence,  $|\alpha_{jm}^k| \ge |\alpha_{in}^k|$  for all (i, n) and k. By multiplying the equation in (B.58) by  $\frac{\partial(\chi w_{pk})}{\partial x_m}$  and integrating over  $\Omega$ , we get

$$\sum_{i,n} \alpha_{in}^{k} \int_{\Omega} Z_{P_{i}^{k},n} \frac{\partial(\chi w_{P_{j}^{k}})}{\partial x_{m}} dx = -\int_{\Omega} \theta_{k} \frac{\partial(\chi w_{P_{j}^{k}})}{\partial x_{m}} dx + \int_{\Omega} L_{\mathbf{P}_{k}}[\phi_{k}] \frac{\partial(\chi w_{P_{j}^{k}})}{\partial x_{m}} dx.$$
(B.59)

First examine the left-hand side of (B.59). By using (B.56)

$$\left|\sum_{i,n} \alpha_{in}^{k} \int_{\Omega} Z_{P_{i}^{k},n} \frac{\partial (\chi w_{P_{j}^{k}})}{\partial x_{m}} dx\right| \ge C \varepsilon_{k}^{N-2} |\alpha_{jm}^{k}|.$$
(B.60)

The first term on the right-hand side of (B.59) can be estimated as

$$\int_{\Omega} \left| \theta_k \frac{\partial(\chi w_{P_j^k})}{\partial x_m} \right| dx \leqslant C \|\theta_k\|_{*,\mathbf{P}_k} \int_{\mathbb{R}^N} |\nabla w_{P_j^k}| dx \leqslant C \varepsilon_k^{N-1} \|\theta_k\|_{*,\mathbf{P}_k}.$$
(B.61)

Finally, by using (A.44) and (B.54),

$$\left| \int_{\Omega} L_{\mathbf{P}_{k}}[\phi_{k}] \frac{\partial(\chi w_{P_{j}^{k}})}{\partial x_{m}} dx \right| = \left| \int_{\Omega} \phi_{k} \left[ -Z_{P_{j}^{k},m} + f'(\chi w_{\mathbf{P}_{k}}) \frac{\partial(\chi w_{P_{j}^{k}})}{\partial x_{m}} \right] dx \right|$$

$$\leq C \|\phi_{k}\|_{*,\mathbf{P}_{k}} \int_{\Omega} \left| \left( f'(w_{\mathbf{P}_{k}}) - f'(w_{P_{j}^{k}}) \right) \frac{\partial w_{P_{j}^{k}}}{\partial x_{m}} \right| dx + C \varepsilon_{k}^{N+2\beta-2} \|\phi_{k}\|_{*,\mathbf{P}_{k}}$$

$$\leq C \varepsilon_{k}^{-1} \|\phi_{k}\|_{*,\mathbf{P}_{k}} \sum_{i \neq j} \int_{\mathbb{R}^{N}} w_{P_{i}^{k}} w_{P_{j}^{k}} dx + C \varepsilon_{k}^{N+2\beta-2} \|\phi_{k}\|_{*,\mathbf{P}_{k}}$$

$$\leq C \|\phi_{k}\|_{*,\mathbf{P}_{k}} (\varepsilon_{k}^{N+2\beta^{2}\sigma-1} + \varepsilon_{k}^{N+2\beta-2})$$

where last inequality follows from Remark A.2. Combining this with (B.59), (B.60) and (B.61), we achieve the thesis.  $\Box$ 

Now we prove the following a priori estimate for (B.58).

**Lemma B.2.** There exists a constant C > 0 such that, provided that  $\varepsilon$  is sufficiently small, if  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$  and  $(\phi, \theta, \alpha_{in})$  satisfies (B.58), the following holds:

$$\|\phi\|_{*,\mathbf{P}} \leqslant C \|\theta\|_{*,\mathbf{P}}.$$

**Proof.** We argue by contradiction. Assume the existence of a sequence  $\varepsilon_k \to 0^+$ ,  $\mathbf{P}_k \in \overline{\Gamma}_{\varepsilon_k}$  and  $(\phi_k, \theta_k, \alpha_{in}^k)$  satisfying (B.58) such that

 $\|\phi_k\|_{*,\mathbf{P}_k} = 1, \qquad \|\theta_k\|_{*,\mathbf{P}_k} = o(1).$ 

By Lemma B.1 we deduce  $\alpha_{in}^k = o(\varepsilon)$  for every (i, n), by which  $\|\theta_k + \sum_{i,n} \alpha_{in}^k Z_{P_i^k, n}\|_{*, \mathbf{P}_k} = o(1)$  and, consequently,

$$\left\|\varepsilon_k^2 \Delta \phi_k - V(x)\phi_k + f'(\chi w_{\mathbf{P}_k})\phi_k\right\|_{*,\mathbf{P}_k} = o(1).$$
(B.62)

We claim that

$$\|\phi_k\|_{L^{\infty}(\bigcup_{i=1}^{\ell} B_{R\varepsilon_k}(P_i^k))} = o(1) \quad \forall R > 0.$$
(B.63)

Otherwise, we may assume that  $\|\phi_k\|_{L^{\infty}(B_{R\varepsilon_k}(P_1^k))} \ge c > 0$  for some R > 0. By multiplying the equation in (B.58) by  $\phi_k$  and integrating by parts we immediately get that the sequence  $\phi_k(\varepsilon_k x + P_1^k)$  is bounded in  $H^1(\mathbb{R}^N)$ . Therefore, possibly passing to a subsequence,  $\phi_k(\varepsilon_k x + P_1^k) \rightarrow \phi_0$  weakly in  $H^1(\mathbb{R}^N)$  and a.e. in  $\mathbb{R}^N$ , and  $\phi_0$  satisfies

 $\Delta\phi_0 - V_0\phi_0 + f'(w)\phi_0 = 0, \quad \left|\phi_0(x)\right| \leqslant w^{-\mu}(x).$ 

According to elliptic regularity theory we may assume  $\phi_k(\varepsilon_k x + P_1^k) \to \phi_0$  uniformly on compact sets, then  $\|\phi_0\|_{\infty} \ge c$ . By assumption (f2)  $\phi_0 = \sum_{n=1}^N a_n \frac{\partial w}{\partial x_n}$ . On the other hand for m = 1, ..., N, using (B.54),

$$0 = \int_{\mathbb{R}^N} \phi_k \left( \varepsilon_k x + P_1^k \right) Z_{P_1^k, m} \left( \varepsilon_k x + P_1^k \right) \to \sum_{n=1}^N a_n \int_{\mathbb{R}^N} \frac{\partial w}{\partial x_n} (V_0 - \Delta) \frac{\partial w}{\partial x_m} = a_m \left\| \frac{\partial w}{\partial x_1} \right\|_{H^1(\mathbb{R}^N)}^2$$

which implies  $a_m = 0$ , that is  $\phi_0 = 0$ . The contradiction follows.

Hence we have proved (B.63), by which we immediately obtain

$$\left\|f'(\chi w_{\mathbf{P}_k})\phi_k\right\|_* \mathbf{P}_k = \mathbf{o}(1)$$

and, by (B.62),

$$\left\|\varepsilon_k^2 \Delta \phi_k - V(x)\phi_k\right\|_{*,\mathbf{P}_k} = \mathrm{o}(1).$$

Next fix R > 0. Observe that by (1.5) it follows that, provided that  $\mu$  is chosen sufficiently small, for every  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$ :

$$\varepsilon^2 \Delta w^{\mu}_{P_i} - V(x) w^{\mu}_{P_i} \leqslant -\frac{V_0}{2} w^{\mu}_{P_i} \quad \text{for } |x - P_i| \geqslant R\varepsilon$$

Then if we set  $\Phi_k(x) = \frac{1}{2} \sum_{i=1}^{\ell} w_{P_i^k}^{\mu}$ , it results

$$\varepsilon_k^2 \Delta(\Phi_k \pm \phi_k) - V(x)(\Phi_k \pm \phi_k) \leq 0 \quad \forall x \in \Omega \setminus \bigcup_{i=1}^{t} B_{R\varepsilon_k}(P_i^k)$$

and, by (B.63),

$$\Phi_k \pm \phi_k \ge 0$$
 if  $|x - P_i^k| = R\varepsilon_k$ .

By the comparison principle it follows that  $\Phi_k \pm \phi_k \ge 0$  in  $\Omega \setminus \bigcup_{i=1}^{\ell} B_{R\varepsilon_k}(P_i^k)$ . Then we have  $|\phi_k| \le \frac{1}{2} \sum_{i=1}^{\ell} w_{P_i^k}^{\mu}$  in  $\Omega \setminus \bigcup_{i=1}^{\ell} B_{R\varepsilon_k}(P_i^k)$ , by which, using (B.63),  $|\phi_k| \le \frac{1}{2} \sum_{i=1}^{\ell} w_{P_i^k}^{\mu}$  in  $\Omega$  for large k, that is  $\|\phi_k\|_{*, \mathbf{P}_k} \le \frac{1}{2}$ , in contradiction with  $\|\phi_k\|_{*, \mathbf{P}_k} = 1$ .  $\Box$ 

Now we are in position to provide the existence of a solution for the system (B.58).

**Lemma B.3.** For  $\varepsilon > 0$  sufficiently small, for every  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$  and  $\theta \in C_{*,\mathbf{P}}$ , there exists a unique pair  $(\phi, \alpha_{in})$  solving (B.58). Furthermore

$$\|\phi\|_{*,\mathbf{P}} \leqslant C \|\theta\|_{*,\mathbf{P}}, \quad |\alpha_{in}| \leqslant C \left( \left( \varepsilon^{2\beta^2\sigma+1} + \varepsilon^{2\beta} \right) \|\theta\|_{*,\mathbf{P}} + \varepsilon \|\theta\|_{*,\mathbf{P}} \right).$$

**Proof.** The existence follows from Fredholm alternative. For every  $\mathbf{P} \in \overline{\Gamma}_{\varepsilon}$  let us consider  $H_{\mathbf{P}}$  the closed subset of  $H_V^1(\Omega)$  defined by

$$H_{\mathbf{P}} = \left\{ \phi \in H_V^1(\Omega) \mid \left( \phi, \frac{\partial(\chi w_{P_i})}{\partial x_n} \right)_{\varepsilon} = 0 \; \forall i = 1, \dots, \ell, \; \forall n = 1, \dots N \right\}.$$

Notice that, by (B.55),  $\phi \in H_{\mathbf{P}}$  solves the equation  $L_{\mathbf{P}}[\phi] = \theta + \sum_{i,n} \alpha_{in} Z_{P_i,n}$  if and only if

$$(\phi,\psi)_{\varepsilon} - \int_{\Omega} f'(\chi w_{\mathbf{P}})\phi\psi \, dx = -\int_{\Omega} \theta\psi \, dx \quad \forall \psi \in H_{\mathbf{P}}.$$
(B.64)

Indeed, once we know  $\phi$ , we can determine the unique  $\alpha_{in}$  from the linear system of equations

$$\int_{\Omega} f'(\chi w_{\mathbf{P}}) \phi \frac{\partial(\chi w_{P_j})}{\partial x_m} dx = \int_{\Omega} \theta \frac{\partial(\chi w_{P_j})}{\partial x_m} dx + \sum_{i,n} \alpha_{in} \int_{\Omega} Z_{P_i,n} \frac{\partial(\chi w_{P_j})}{\partial x_m} dx,$$

for  $j = 1, ..., \ell$ , m = 1, ..., N, which is uniquely solvable according to (B.56). By standard elliptic regularity,  $\phi \in H^2(\Omega)$ .

Thus it remains to solve (B.64). According to Riesz's representation theorem, take  $K_{\mathbf{P}}(\phi), \overline{\theta} \in H_{\mathbf{P}}$  such that

$$\left(K_{\mathbf{P}}(\phi),\psi\right)_{\varepsilon} = -\int_{\Omega} f'(\chi w_{\mathbf{P}})\phi\psi\,dx \qquad (\bar{\theta},\psi)_{\varepsilon} = -\int_{\Omega} \theta\psi\,dx \quad \forall\psi\in H_{\mathbf{P}}$$

Then problem (B.64) consists in finding  $\phi \in H_{\mathbf{P}}$  such that

$$\phi + K_{\mathbf{P}}(\phi) = \bar{\theta}. \tag{B.65}$$

It is easy to prove that  $K_{\mathbf{P}}$  is a linear compact operator from  $H_{\mathbf{P}}$  to  $H_{\mathbf{P}}$ . Using Fredholm's alternatives, (B.65) has a unique solution for each  $\overline{\theta}$ , if and only if (B.65) has a unique solution for  $\overline{\theta} = 0$ . Let  $\phi \in H_{\mathbf{P}}$  be a solution of  $\phi + K_{\mathbf{P}}(\phi) = 0$ ; then  $\phi$  solves the system (B.58) with  $\theta = 0$  for some  $\alpha_{in} \in \mathbb{R}$ . Lemma B.2 implies  $\phi \equiv 0$ . The remaining part of the lemma follow by Lemmas B.1 and B.2.  $\Box$ 

#### B.2. Lyapunov–Schmidt reduction

**Proof of Lemma 2.1.** We write the equation in (2.9) in the following form:

$$L_{\mathbf{P}}[\phi] = -S_{\varepsilon}[\chi w_{\mathbf{P}}] - N_{\mathbf{P}}[\phi] + \sum_{i,n} \alpha_{in} Z_{P_{i},n}$$
(B.66)

and use contraction mapping theorem. Here

$$N_{\mathbf{P}}[\phi] = f(\chi w_{\mathbf{P}} + \phi) - f(\chi w_{\mathbf{P}}) - f'(\chi w_{\mathbf{P}})\phi.$$

Consider the metric space  $\mathscr{B}_{\mathbf{P}} = \{\phi \in \mathscr{C}(\overline{\Omega}) \mid \|\phi\|_{*,\mathbf{P}} \leq \varepsilon^{\tau}\}$  endowed with the norm  $\|\cdot\|_{*,\mathbf{P}}$ . Taken  $\phi_1, \phi_2 \in \mathscr{B}_{\mathbf{P}}$ , by assumption (f1) we have

$$\left\| N_{\mathbf{P}}[\phi_1] - N_{\mathbf{P}}[\phi_2] \right\|_{*,\mathbf{P}} \leqslant C \varepsilon^{\sigma \tau} \|\phi_1 - \phi_2\|_{*,\mathbf{P}}.$$
(B.67)

For every  $\phi \in \mathscr{B}_{\mathbf{P}}$  we define  $\mathscr{A}_{\mathbf{P}}[\phi] \in H^2(\Omega) \cap H^1_V(\Omega)$  to be the unique solution to the system (B.58) given by Lemma B.3 with  $\theta = \theta_{\mathbf{P}}[\phi] := -S_{\varepsilon}[\chi w_{\mathbf{P}}] - N_{\mathbf{P}}[\phi]$ . By (B.67), Lemmas A.4, B.3 and the choice of  $\tau$ 

$$\left\|\mathscr{A}_{\mathbf{P}}[\phi]\right\|_{*,\mathbf{P}} \leq C \left\|\theta_{\mathbf{P}}[\phi]\right\|_{*,\mathbf{P}} \leq C \left(\varepsilon^{\beta^{2}(\beta^{2}+\sigma)} + \varepsilon^{(1+\sigma)\tau}\right) < \varepsilon^{\tau}$$

at least for small  $\varepsilon$ , and hence  $\mathscr{A}_{\mathbf{P}}[\phi] \in \mathscr{B}_{\mathbf{P}}$ . Moreover, since  $\mathscr{A}_{\mathbf{P}}[\phi_1] - \mathscr{A}_{\mathbf{P}}[\phi_2]$  solves the system (B.58) with  $\theta = -N_{\mathbf{P}}[\phi_1] + N_{\mathbf{P}}[\phi_2]$ , by (B.67) and Lemma B.3 we also have that

$$\left\|\mathscr{A}_{\mathbf{P}}[\phi_{1}] - \mathscr{A}_{\mathbf{P}}[\phi_{2}]\right\|_{*,\mathbf{P}} \leqslant C \left\|N_{\mathbf{P}}[\phi_{1}] - N_{\mathbf{P}}[\phi_{2}]\right\|_{*,\mathbf{P}} < \|\phi_{1} - \phi_{2}\|_{*,\mathbf{P}} \quad \forall \phi_{1}, \phi_{2} \in \mathscr{B}_{\mathbf{P}}, \ \forall \mathbf{P} \in \overline{\Gamma}_{\varepsilon},$$

i.e. the map  $\mathscr{A}_{\mathbf{P}}$  is a contraction map from  $\mathscr{B}_{\mathbf{P}}$  to  $\mathscr{B}_{\mathbf{P}}$ . By the contraction mapping theorem, (2.9) has a unique solution  $(\phi_{\mathbf{P}}, \alpha_{in}(\mathbf{P})) \in \mathscr{B}_{\mathbf{P}} \times \mathbb{R}^{N\ell}$ .

Finally, by multiplying the equation in (B.66) by  $\phi_{\mathbf{P}}$  and integrating over  $\Omega$  we immediately get  $(\phi_{\mathbf{P}}, \phi_{\mathbf{P}})_{\varepsilon} \leq C\varepsilon^{N+2\tau}$ . By Lemma B.1 we get

$$\left|\alpha_{in}(\mathbf{P})\right| \leqslant C\left(\left(\varepsilon^{2\beta^{2}\sigma+1}+\varepsilon^{2\beta}\right)\|\phi_{\mathbf{P}}\|_{*,\mathbf{P}}+\varepsilon\left\|\theta_{\mathbf{P}}[\phi_{\mathbf{P}}]\right\|_{*,\mathbf{P}}\right) \leqslant \varepsilon^{1+\tau}.$$

To prove that the map  $\mathbf{P} \in \Gamma_{\varepsilon} \to \phi_{\mathbf{P}} \in H^1_V(\Omega)$  is  $\mathscr{C}^1$ , consider the following map  $\Psi : \Gamma_{\varepsilon} \times H^1_V(\Omega) \times \mathbb{R}^{N\ell} \to H^1_V(\Omega) \times \mathbb{R}^{N\ell}$ :

$$\Psi(\mathbf{P},\phi,\alpha_{in}) = \begin{pmatrix} (V(x) - \varepsilon^2 \Delta)^{-1} (S_{\varepsilon}[\chi w_{\mathbf{P}} + \phi]) - \sum_{i,n} \alpha_{in} \frac{\partial(\chi w_{P_i})}{\partial x_n} \\ \int_{\Omega} \phi Z_{P_i,n} \, dx \end{pmatrix},$$
(B.68)

where  $v = (V(x) - \varepsilon^2 \Delta)^{-1}(h)$  is defined as the unique solution in  $H_V^1(\Omega)$  of  $V(x)v - \varepsilon^2 \Delta v = h$ . It is immediate that  $(\phi, \alpha_{in})$  solves the system (2.9) if and only if  $\Psi(\mathbf{P}, \phi, \alpha_{in}) = 0$ . The thesis will easily follow from the Implicit Function Theorem.  $\Box$ 

Proof of Proposition 2.2. We compute

$$J_{\varepsilon}[\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}] = \frac{1}{2} \int_{\Omega} \left( \varepsilon^{2} |\nabla(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}})|^{2} + V(x)(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}})^{2} \right) dx - \int_{\Omega} F(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}) dx$$
$$= J_{\varepsilon}[\chi w_{\mathbf{P}}] - \int_{\Omega} S_{\varepsilon}[\chi w_{\mathbf{P}}] \phi_{\mathbf{P}} dx + \frac{1}{2} (\phi_{\mathbf{P}}, \phi_{\mathbf{P}})_{\varepsilon}$$
$$- \int_{\Omega} \left( F(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}) - F(\chi w_{\mathbf{P}}) - f(\chi w_{\mathbf{P}}) \phi_{\mathbf{P}} \right) dx$$

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ . By Lemma A.4 we have  $|S_{\varepsilon}[\chi w_{\mathbf{P}}]| \leq \varepsilon^{\tau} \sum_{i=1}^{\ell} w_{P_i}^{1-\beta^2}$  for small  $\varepsilon$ , while  $|F(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}) - F(\chi w_{\mathbf{P}}) - f(\chi w_{\mathbf{P}})\phi_{\mathbf{P}}| \leq C |\phi_{\mathbf{P}}|^2$ ; hence, by using (2.11) we get

 $J_{\varepsilon}[\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}] = J_{\varepsilon}[\chi w_{\mathbf{P}}] + \mathcal{O}(\varepsilon^{N+2\tau})$ 

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ . (2.12) follows from Proposition A.6, observing that  $2\tau = 2\beta^4(1+\sigma) > 2$  if  $\beta$  is sufficiently closed to 1. Next, denoting by  $P_i^n$  the *n*th component of  $P_i$ , since  $\frac{\partial w_{\mathbf{P}}}{\partial P_i^n} = -\lambda_i \frac{\partial w_{P_i}}{\partial x_n}$ , we compute

$$\begin{split} \frac{\partial}{\partial P_i^n} J_{\varepsilon}[\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}] &= -\int_{\Omega} S_{\varepsilon}[\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}] \frac{\partial(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}})}{\partial P_i^n} dx \\ &= \frac{\partial}{\partial P_i^n} J_{\varepsilon}[\chi w_{\mathbf{P}}] - \lambda_i \left(\phi_{\mathbf{P}}, \frac{\partial(\chi w_{P_i})}{\partial x_n}\right)_{\varepsilon} - \int_{\Omega} S_{\varepsilon}[\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}] \frac{\partial\phi_{\mathbf{P}}}{\partial P_i^n} \\ &- \int_{\Omega} \left(f(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}) - f(\chi w_{\mathbf{P}})\right) \frac{\partial(\chi w_{\mathbf{P}})}{\partial P_i^n} \\ &= \frac{\partial}{\partial P_i^n} J_{\varepsilon}[\chi w_{\mathbf{P}}] - \sum_{j,m} \alpha_{jm}(\mathbf{P}) \int_{\Omega} Z_{P_j,m} \frac{\partial\phi_{\mathbf{P}}}{\partial P_i^n} + \lambda_i \int_{\Omega} \left(f(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}) - f(\chi w_{\mathbf{P}})\right) \chi \frac{\partial w_{P_i}}{\partial x_n}. \end{split}$$

Since  $\int_{\Omega} Z_{P_i,m} \phi_{\mathbf{P}} dx = 0$ , by differentiation we get<sup>5</sup>

$$\int_{\Omega} Z_{P_j,m} \frac{\partial \phi_{\mathbf{P}}}{\partial P_i^n} dx = -\int_{\Omega} \frac{\partial Z_{P_j,m}}{\partial P_i^n} \phi_{\mathbf{P}} = O(\varepsilon^{N+\tau-2}),$$
(B.69)

by which, using Lemma 2.1,

$$\sum_{j,m} \alpha_{jm}(\mathbf{P}) \int_{\Omega} Z_{P_j,m} \frac{\partial \phi_{\mathbf{P}}}{\partial P_i^n} dx = O(\varepsilon^{N+2\tau-1}).$$
(B.70)

<sup>5</sup> Observe that 
$$\left|\frac{\partial Z_{P_j,m}}{\partial P_i^n}\right| = \delta_{ij} \left| (V(x) - \varepsilon^2 \Delta) \left(\frac{\partial}{\partial x_n} \left(\chi \frac{\partial w_{P_i}}{\partial x_m}\right) \right) \right| \leq C \varepsilon^{-2} w_{P_i} \text{ by (1.5).}$$

By assumption (f1) we have  $|f(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}) - f(\chi w_{\mathbf{P}}) - f'(\chi w_{\mathbf{P}})\phi_{\mathbf{P}}| \leq C |\phi_{\mathbf{P}}|^{1+\sigma}$ ; consequently

$$\int_{\Omega} \left( f(\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}) - f(\chi w_{\mathbf{P}}) - f'(\chi w_{\mathbf{P}})\phi_{\mathbf{P}} \right) \chi \frac{\partial w_{P_i}}{\partial x_n} = O(\varepsilon^{N + \tau(1 + \sigma) - 1}).$$
(B.71)

Finally, by (A.43), (A.44) and (B.54),

$$\left| \int_{\Omega} f'(\chi w_{\mathbf{P}}) \phi_{\mathbf{P}} \chi \frac{\partial w_{P_i}}{\partial x_n} \right| = \left| \int_{\Omega} \left( f'(\chi w_{\mathbf{P}}) \chi \frac{\partial w_{P_i}}{\partial x_n} - Z_{P_i,n} \right) \phi_{\mathbf{P}} dx \right|$$
$$\leq C \varepsilon^{\tau} \int_{\Omega} \left| f'(w_{\mathbf{P}}) - f'(w_{P_i}) \right| \left| \frac{\partial w_{P_i}}{\partial x_n} \right| dx + C \varepsilon^{N+2\beta+\tau-1}$$
$$\leq C \varepsilon^{\tau} \sum_{j \neq i} \int_{\Omega} w_{P_j}^{\sigma} \left| \frac{\partial w_{P_i}}{\partial x_n} \right| dx + C \varepsilon^{N+2\beta+\tau-1} \leq C \varepsilon^{N+2\beta^2\sigma+\tau-1}$$
(B.72)

where we have used Lemma A.2. Combining (B.70)-(B.72), we deduce

$$\frac{\partial}{\partial P_i^n} J_{\varepsilon}[\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}] = \frac{\partial}{\partial P_i^n} J_{\varepsilon}[\chi w_{\mathbf{P}}] + \mathcal{O}(\varepsilon^{N + \beta^4 (1 + \sigma)^2 - 1})$$

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ . By applying Proposition A.6 we obtain (2.13), using that  $\beta^4 (1+\sigma)^2 - 1 > 2\beta - 1$  by assumption (f1) if  $\beta$  is closed to 1.  $\Box$ 

Remark B.4. By the proof of Proposition 2.2 it follows that

$$\nabla_{\mathbf{P}} M_{\varepsilon}[\mathbf{P}] = \varepsilon^{-N} \nabla_{\mathbf{P}} J_{\varepsilon}[\chi w_{\mathbf{P}}] + \mathcal{O}(\varepsilon^{\beta^4(1+\sigma)^2 - 1})$$

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ . According to assumption (f1) we have  $\beta^4 (1 + \sigma)^2 - 1 > 2\beta \frac{l-1}{l}$  if  $\beta$  is sufficiently closed to 1. Therefore we have

$$\nabla_{\mathbf{P}} M_{\varepsilon}[\mathbf{P}] = \varepsilon^{-N} \nabla_{\mathbf{P}} J_{\varepsilon}[\chi w_{\mathbf{P}}] + o\left(\varepsilon^{2\beta \frac{l-1}{l}}\right)$$
(B.73)

uniformly for  $\mathbf{P} \in \Gamma_{\varepsilon}$ .

**Proof of Proposition 2.3.** We may assume, up to a subsequence,  $\lim_{k\to\infty} \varepsilon_k^{-2\beta}(V(P_1^k) - V_0) > 0$  and

$$\lim_{k \to \infty} \frac{|P_i^k - P_1^k|}{\varepsilon_k \log \frac{1}{\varepsilon_k}} < +\infty \quad \forall i = 1, \dots, \ell', \qquad \frac{|P_i^k - P_1^k|}{\varepsilon_k \log \frac{1}{\varepsilon_k}} \to +\infty \quad \forall i = \ell' + 1, \dots, \ell$$
(B.74)

for some  $1 \leq \ell' \leq \ell$ . Assume  $\frac{P_1^k - P_0}{|P_1^k - P_0|} \rightarrow Q$  and set  $\mathbf{Q} = (\underbrace{Q, \dots, Q}_{\ell'}, 0, \dots, 0) \in \mathbb{R}^{N\ell}$ ; observe that  $\frac{d}{dt} w_{\mathbf{P}^k + t\mathbf{Q}}|_{t=0} = \underbrace{Q, \dots, Q}_{\ell'}$ .

$$-\sum_{i=1}^{\ell'}\lambda_i \nabla w_{P_i^k} \cdot Q$$
, by which

$$\begin{aligned} \frac{d}{dt} J_{\varepsilon_{k}}[\chi w_{\mathbf{P}^{k}+t\mathbf{Q}}]|_{t=0} &= -\left\langle J_{\varepsilon_{k}}'[\chi w_{\mathbf{P}^{k}}], \sum_{i=1}^{\ell'} \lambda_{i} \chi \nabla w_{P_{i}^{k}} \cdot Q \right\rangle \\ &= \sum_{i=1}^{\ell'} \lambda_{i} \int_{\Omega} \left( \varepsilon_{k}^{2} \Delta(\chi w_{\mathbf{P}^{k}}) - V(x) \chi w_{\mathbf{P}^{k}} + f(\chi w_{\mathbf{P}^{k}}) \right) \chi \nabla w_{P_{i}^{k}} \cdot Q \, dx \\ &= \sum_{i=1}^{\ell'} \lambda_{i} \int_{\mathbb{R}^{N}} \left( \varepsilon_{k}^{2} \Delta w_{\mathbf{P}^{k}} - V(x) \chi w_{\mathbf{P}^{k}} + f(w_{\mathbf{P}^{k}}) \right) \nabla w_{P_{i}^{k}} \cdot Q \, dx + o(\varepsilon_{k}^{N+2}) \end{aligned}$$

by (A.43)-(A.44). By (1.5) we deduce

$$w_{P_j^k} |\nabla w_{P_i^k}|, \varepsilon_k^2 \Delta w_{P_j^k} |\nabla w_{P_i^k}| \leqslant C \varepsilon_k^{-1} e^{-\sqrt{V_0} \frac{|P_i^k - P_j^k|}{\varepsilon_k}} = o(\varepsilon_k^2) \quad \forall i \leqslant \ell', \ j > \ell',$$

which implies

$$\frac{d}{dt} J_{\varepsilon_k} [\chi w_{\mathbf{P}^k + t\mathbf{Q}}] \Big|_{t=0} = \int_{\mathbb{R}^N} \left[ \sum_{j=1}^{\ell'} \lambda_j (\varepsilon_k^2 \Delta w_{P_j^k} - V(x)\chi w_{P_j^k}) + f\left(\sum_{j=1}^{\ell'} \lambda_j w_{P_j^k}\right) \right] \sum_{i=1}^{\ell'} \lambda_i \nabla w_{P_i^k} \cdot Q \, dx + \mathbf{o}(\varepsilon_k^{N+2}) \\
= \frac{d}{dt} I_{\varepsilon_k} \left[ \sum_{j=1}^{\ell'} \lambda_j w_{P_j^k + tQ} \right] \Big|_{t=0} - \int_{\mathbb{R}^N} (\chi V(x) - V_0) \left( \sum_{j=1}^{\ell'} \lambda_j w_{P_j^k} \right) \left( \sum_{i=1}^{\ell'} \lambda_i \nabla w_{P_i^k} \cdot Q \right) dx + \mathbf{o}(\varepsilon_k^{N+2})$$

where we have set  $I_{\varepsilon}(v) = \frac{\varepsilon^2}{2} \int_{\mathbb{R}^N} |\nabla v|^2 dx + \frac{V_0}{2} \int_{\mathbb{R}^N} |v|^2 dx - \int_{\mathbb{R}^N} F(v) dx$ . Since  $I_{\varepsilon}$  is translation invariant we have  $\frac{d}{dt} I_{\varepsilon} [\sum_{j=1}^{\ell'} \lambda_j w_{P_j^k + tQ}] = 0$ ; we arrive at

$$\frac{d}{dt}J_{\varepsilon_k}[\chi w_{\mathbf{P}^k+t\mathbf{Q}}]\Big|_{t=0} = -\int\limits_{\mathbb{R}^N} \left(\chi V(x) - V_0\right) \left(\sum_{j=1}^{\ell'} \lambda_j w_{P_j^k}\right) \left(\sum_{i=1}^{\ell'} \lambda_i \nabla w_{P_i^k} \cdot Q\right) dx + o(\varepsilon_k^{N+2}).$$

Using (A.45) and Remark A.2, for  $i \neq j$  we have

$$\int_{\mathbb{R}^N} \left( \chi V(x) - V_0 \right) w_{P_j^k} |\nabla w_{P_i^k}| \, dx \leqslant C \varepsilon_k^{2\beta - 1} \int_{\mathbb{R}^N} w_{P_j^k}^{2/3} w_{P_i^k} \, dx \leqslant C \varepsilon_k^{N + 2\beta + \frac{4}{3}\beta^2 - 1}$$

Therefore, if  $\beta$  is sufficiently closed to 1,

$$\begin{aligned} \frac{d}{dt} J_{\varepsilon_k}[\chi w_{\mathbf{P}^k + t\mathbf{Q}}] \bigg|_{t=0} &= -\int\limits_{\mathbb{R}^N} \left( \chi V(x) - V_0 \right) \left( \sum_{i=1}^{\ell'} w_{P_i^k} \nabla w_{P_i^k} \cdot Q \right) dx + \mathbf{o}(\varepsilon_k^{N+2}) \\ &= \frac{1}{2} \int\limits_{\mathbb{R}^N} \left( \sum_{i=1}^{\ell'} w_{P_i^k}^2 \nabla (\chi V(x)) \cdot Q \right) dx + \mathbf{o}(\varepsilon_k^{N+2}). \end{aligned}$$

Observe that, since  $V \in \mathscr{C}^2(\Lambda)$ , for every  $i = 1, ..., \ell'$ 

$$\nabla(\chi V(x)) - \nabla V(P_i^k) - D^2 V(P_i^k) (x - P_i^k) |w_{P_i^k} \leq C |x - P_i^k|^2 w_{P_i^k} \leq C \varepsilon_k^2 w_{P_i^k}^{1/2}$$

by which, since  $\int_{\mathbb{R}^N} D^2 V(P_i^k) (x - P_i^k) Q w_{P_i^k}^2 dx = \varepsilon_k^N \int_{\mathbb{R}^N} D^2 V(P_i^k) y Q w^2 dy = 0$ ,

$$\frac{d}{dt} J_{\varepsilon}[\chi w_{\mathbf{P}^{k}+t\mathbf{Q}}]\Big|_{t=0} = c_{2}\varepsilon_{k}^{N} \sum_{i=1}^{\ell'} \nabla V(P_{i}^{k}) \cdot Q + \mathcal{O}(\varepsilon_{k}^{N+2}) = c_{2}\varepsilon_{k}^{N} \sum_{i=1}^{\ell} \nabla V(P_{i}^{k}) \cdot Q_{i} + \mathcal{O}(\varepsilon_{k}^{N+2}).$$

Since  $V(P_1^k) \ge C\varepsilon_k^{2\beta}$ , then  $|P_1^k - P_0| \ge C\varepsilon_k^{\beta}$  and, by (B.74),  $|P_i^k - P_0| \ge C\varepsilon_k^{\beta}$  for every  $i = 1, ..., \ell'$ , hence

$$\left|\frac{P_i^k - P_0}{|P_i^k - P_0|} - \frac{P_1^k - P_0}{|P_1^k - P_0|}\right| \leqslant \left(\frac{1}{|P_i^k - P_0|} + \frac{1}{|P_1^k - P_0|}\right) |P_i^k - P_1^k| \leqslant C\varepsilon_k^{1-\beta} \log \frac{1}{\varepsilon_k};$$

we deduce  $\frac{P_i^k - P_0}{|P_i^k - P_0|} \to Q$  for every  $i = 1, \dots, \ell'$ . Therefore

$$\frac{d}{dt} J_{\varepsilon}[\chi w_{\mathbf{P}^{k}+t\mathbf{Q}}]\Big|_{t=0} = c_{2}\varepsilon_{k}^{N} \sum_{i=1}^{\ell'} \nabla V(P_{i}^{k}) \cdot \frac{P_{i}^{k} - P_{0}}{|P_{i}^{k} - P_{0}|} (1 + o(1)) + O(\varepsilon_{k}^{N+2})$$

and (2.14) follows from Remarks 1.2 and B.4. Finally observe that

$$\nabla_{\mathbf{P}}\left[w\left(\frac{P_i-P_j}{\varepsilon_k}\right)\right]\Big|_{\mathbf{P}=\mathbf{P}_k}\cdot\mathbf{Q}=0 \quad \text{if } i,j\leqslant\ell' \text{ or } i,j>\ell',$$

while, if  $i \leq \ell' < j$ ,

$$\nabla_{\mathbf{P}} \left[ w \left( \frac{P_i - P_j}{\varepsilon_k} \right) \right] \Big|_{\mathbf{P} = \mathbf{P}_k} \cdot \mathbf{Q} = \frac{d}{dt} w \left( \frac{P_i^k + t Q - P_j^k}{\varepsilon_k} \right) \Big|_{t=0} = O\left(\varepsilon_k^{-1} e^{-\sqrt{V_0} \frac{|P_i^k - P_j^k|}{\varepsilon_k}}\right) = o\left(\varepsilon_k^2\right)$$

by (B.74). □

**Proof of Lemma 2.4.** Fix  $\varepsilon_0 > 0$  sufficiently small such that Lemma 2.1 holds for  $\varepsilon \in (0, \varepsilon_0)$ . According to Lemma 2.1, for every  $\varepsilon \in (0, \varepsilon_0)$  and  $\mathbf{P} = (P_1, \dots, P_\ell) \in \overline{\Gamma}_{\varepsilon} \phi_{\mathbf{P}}$  solves the equation

$$S_{\varepsilon}[\chi w_{\mathbf{P}} + \phi_{\mathbf{P}}] = \sum_{i,n} \alpha_{in}(\mathbf{P}) Z_{P_{i,n}} \quad \text{in } \Omega.$$
(B.75)

Let  $\mathbf{P}_{\varepsilon} \in \Gamma_{\varepsilon}$  be a critical point of  $M_{\varepsilon}$ :

$$\frac{\partial}{\partial P_j^m}\Big|_{\mathbf{P}=\mathbf{P}_{\varepsilon}} M_{\varepsilon}[\mathbf{P}] = 0, \quad j = 1, \dots, \ell, \ m = 1, \dots, N,$$
(B.76)

where  $P_j^m$  denotes the *m*th component of  $P_j$ . Using the  $\mathscr{C}^1$  regularity of the map  $\mathbf{P} \in \Gamma_{\varepsilon} \mapsto \phi_{\mathbf{P}} \in H_V^1(\Omega)$ , (B.76) may be rewritten as

$$\int_{\Omega} \left( \varepsilon^2 \nabla v_{\varepsilon} \nabla \frac{\partial (\chi w_{\mathbf{P}} + \phi_{\mathbf{P}})}{\partial P_j^m} + \left( V(x) v_{\varepsilon} - f(v_{\varepsilon}) \right) \frac{\partial (\chi w_{\mathbf{P}} + \phi_{\mathbf{P}})}{\partial P_j^m} \right) dx \bigg|_{\mathbf{P} = \mathbf{P}_{\varepsilon}} = 0,$$

which is equivalent, by (B.75), to

$$\sum_{i,n} \alpha_{in}(\mathbf{P}_{\varepsilon}) \int_{\Omega} Z_{P_i,n} \frac{\partial (\chi w_{\mathbf{P}} + \phi_{\mathbf{P}})}{\partial P_j^m} dx \bigg|_{\mathbf{P} = \mathbf{P}_{\varepsilon}} = 0.$$

Since  $\frac{\partial w_{\mathbf{P}}}{\partial P_{j}^{m}} = -\frac{\partial w_{P_{j}}}{\partial x_{m}}$ , using (B.56) and the estimate obtained in (B.69) we achieve

$$\alpha_{jm}(\mathbf{P}_{\varepsilon}) \left\| \frac{\partial w}{\partial x_1} \right\|_{H^1(\mathbb{R}^N)}^2 + \sum_{i,n} \mathrm{o}(1) \alpha_{in}(\mathbf{P}_{\varepsilon}) = 0.$$

So  $\alpha_{jm}(\mathbf{P}_{\varepsilon}) = 0$  for  $j = 1, ..., \ell, m = 1, ..., N$ , and the thesis follows.  $\Box$ 

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