ARBITRARY MANY BOUNDARY PEAK SOLUTIONS FOR AN ELLIPTIC NEUMANN PROBLEM WITH CRITICAL GROWTH

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ABSTRACT. We consider the following problem

$$-\Delta u + \mu u = u^{2^*-1},\ u > 0 \text{ in } \Omega, \quad \frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega,$$

where $\mu > 0$ is a large parameter, Ω is a bounded domain in $\mathbb{R}^N$, $N \geq 3$ and $2^* = 2N/(N-2)$. Let $H(P)$ be the mean curvature function of the boundary. Assuming that $H(P)$ has a local minimum point with positive minimum, then for any integer k, the above problem has a $k-$boundary peaks solution. As a consequence, we show that if Ω is *strictly convex*, then the above problem has arbitrarily many solutions, provided that μ is large.

Résumé: On considère le problème suivant:

$$-\Delta u + \mu u = u^{2^*-1},\ u > 0 \text{ dans } \Omega, \quad \frac{\partial u}{\partial n} = 0 \text{ sur } \partial\Omega,$$

où $\mu > 0$ est un grand paramètre, Ω est un domaine borné de $\mathbb{R}^N$, $N \geq 3$ et $2^* = 2N/(N-2)$. Soit $H(P)$ la courbure moyenne, supposons que H admet un minimum local à valeur strictement positive, alors pour tout $k \in \mathbb{N}$, le problème de Neumann ci-dessus a une solution avec k pics sur le bord. Par conséquent, on montre que si Ω est *strictement convexe*, le problème a un nombre arbitraire de solutions, à condition que μ soit suffisamment grand.

Keywords: Critical Exponent; Boundary Peaks; Singularly Perturbed Neumann Problem; Gradient Flows

1. Introduction

In this paper, we study the following nonlinear elliptic Neumann problem:

$$(P_{q,\mu}) \qquad \begin{cases} -\Delta u + \mu u &= u^q, \quad u > 0, \qquad \text{in } \Omega, \\ \frac{\partial u}{\partial n} &= 0, \qquad\qquad\qquad \text{on } \partial\Omega, \end{cases}$$

where $q = \frac{N+2}{N-2}$, $\mu > 0$, Ω is a smooth and bounded domain in $\mathbb{R}^N, N \geq 3$ and n is the outward unit normal of $\partial\Omega$ at y.

Equation $(P_{q,\mu})$ arises in many branches of the applied sciences. For example, it can be viewed as a steady-state equation for the shadow system of the Gierer-Meinhardt system in biological pattern formation ([13], [24]), or of parabolic equations in chemotaxis, e.g. Keller-Segel model ([22]).

When q is subcritical, i.e. $q < \frac{N+2}{N-2}$, Lin, Ni and Takagi [22] proved that the only solution, for small μ, is the constant one, whereas nonconstant solutions appear for large μ, which blow up, as μ goes to infinity, at one or several points. The least energy solution blows up at a boundary point which maximizes the mean curvature of the boundary [26][27]. (From now on, we denote the mean curvature function by $H(P)$, $P \in \partial\Omega$.) Higher energy solutions exist which blow up at one or several points, located on the boundary [5][10] [9] [12][20][21][38], or in the interior of the domain [6][11][16][18], or some of them on the boundary and others in the interior [19]. (A review up to 2004 can be found in [24].) In particular, we mention the following result which proves the existence of arbitrarily many boundary spikes.

Theorem A ([20]). *Suppose that $1 < q < \frac{N+2}{N-2}$ and that $Q_0 \in \partial\Omega$ is a local minimum point of the mean curvature function $H(P)$. Then given any positive integer k, there exists a $\mu_k > 0$ such that for $\mu > \mu_k$, problem $(P_{q,\mu})$ has a solution u_μ with k spikes $Q_j^\mu, j = 1, ..., k$ such that $Q_j^\mu \in \partial\Omega, Q_j^\mu \to Q_0$ and $|Q_i^\mu - Q_j^\mu| \geq C\frac{1}{\sqrt{\mu}}\log\mu$. As a corollary, for any fixed $k \geq 1$, there exists $\mu > \mu_k$ such that $(P_{q,\mu})$ has a k boundary-peaked solution*

In the critical case, i.e. $q = \frac{N+2}{N-2}$, there also have been many works on $(P_{q,\mu})$. For large μ, nonconstant solutions exist [1][34]. As in the subcritical case, the least energy solution blows up, as μ goes to infinity, at a point which maximizes the mean curvature of the boundary [4][25]. Considering higher energy solutions, Adimurthi, Mancini and Yadava [3], showed that for $N \geq 6$, single boundary peak exists at a nondegenerate critical point of the mean curvature function with positive values. Rey generalized this result to the case $N = 3$ [29].

However, in contrast to the subcritical case, the results on solutions with multiple peaks in the critical case have been very limited. For the very special case when the domain has certain symmetries, Wang in [35]-[37] restricted his consideration to the symmetric Sobolev space and showed that there exists a solution with multiple peaks (of related symmetry) for the critical case. On the other hand, Grossi [15] showed that for a *strictly convex domain* Ω, the existence of a solution which has approximately twice as much energy as a *least energy* solution and therefore it might possess two peaks on the boundary. Using variational methods, Ghoussoub and Gui [14] constructed k (separated) boundary peaks at k (separated) *local maximum points* of $H(P)$, provided $N \geq 5$ and $H > 0$. Adimurthi, Mancini and Yadava [3] and Rey [30] constructed multiple peak solutions at multiple nondegenerate critical points of $H(P)$ for $N \geq 6$ (and for $N = 3$ at [29]). In all the above papers, it is assumed that $H > 0$. This has been proved to be necessary by Gui and Lin [17], and Rey [30].

Our aim, in this paper, is to prove a version of Theorem A, in the critical exponent case, for *all dimensions.* Namely, we consider the following problem

$$\begin{cases} -\Delta u + \mu u = u^{2^*-1}, \ u > 0 & \text{in } \Omega \\ \frac{\partial u}{\partial n} = 0, & \text{on } \partial\Omega, \end{cases} \tag{1.1}$$

where $\mu > 0$ is a large parameter, Ω is a bounded domain in $\mathbb{R}^N$, $N \geq 3$ and $2^* = 2N/(N-2)$. Our main result can be stated as follows: *assuming that $H(P)$ has a local minimum point with positive minimum, then for any integer k, problem (1.1) has a $k-$boundary peaks* *solution. As a consequence, we prove that if Ω is strictly convex, then (1.1) has arbitrarily many solutions.*

To make it more precise, we define the energy functional corresponding to (1.1) to be

$$I(u)=\frac{1}{2}\int_\Omega\big(|\nabla u|^2+\mu u^2\big)\,dy-\frac{1}{2^*}\int_\Omega|u|^{2^*}\,dy,\quad u\in H^1(\Omega).$$

For any $\bar{x}\in\mathbb{R}^N$, $\bar\lambda>0$, we denote

$$U_{\bar x,\bar\lambda}(y)=\frac{c_0\bar\lambda^{(N-2)/2}}{(1+\bar\lambda^2|y-\bar x|^2)^{(N-2)/2}},\tag{1.2}$$

where $c_0=\big[N(N-2)\big]^{(N-2)/4}$. Then $U_{\bar x,\bar\lambda}$ satisfies $-\Delta U_{\bar x,\bar\lambda}=U_{\bar x,\bar\lambda}^{2^*-1}$. In this paper, we will use the following notation: $U=U_{0,1}$.

To find a solution for (1.1) with sharp peaks, the first step is to construct an approximate solution. The first obvious choice for the approximate solution is $U_{\bar x,\bar\lambda}$. It turns out that this choice works if $N\ge 5$. In the lower dimension $N=3,4$, the function $U_{\bar x,\bar\lambda}$ does not concentrate fast enough, so the error term is not small to yield a solution. See Remark 2.2. For this reason, we need to modify $U_{\bar x,\bar\lambda}$ in the case $N=3,4$. We define the approximate solution as follows.

Let

$$V_{\bar x,\bar\lambda}=U_{\bar x,\bar\lambda},\quad \text{if } N\ge 5.$$

If $N=3$, we use the approximate solution as in [29]

$$V_{\bar x,\bar\lambda}(y)=U_{\bar x,\bar\lambda}(y)-\frac{c_0}{\bar\lambda^{1/2}|y-\bar x|}\big(1-e^{-\sqrt{\mu}|y-\bar x|}\big),\quad \text{if } N=3.$$

For the case $N=4$, let $V_{\bar x,\bar\lambda}$ be the solution of

$$-\Delta u+\mu u=U_{\bar x,\bar\lambda}^{2^*-1},\text{in }\mathbb{R}^4,\quad u(y)\to 0,\text{as }|y|\to+\infty.\tag{1.3}$$

For any $u,v\in H^1(\Omega)$, we define

$$\langle u,v\rangle=\int_\Omega\big(\nabla u\cdot\nabla v+\mu uv\big)\,dy,\quad \|u\|=\langle u,u\rangle^{1/2}.$$

The main result of this paper is the following:

Theorem 1.1. *Suppose that there is a set $S\subset\partial\Omega$, such that $0<\min_{x\in S}H(x)<\min_{x\in\partial S}H(x)$. Then, for any integer $k\ge 1$, there is an $\mu_k>0$, depending on k, such that for any $\mu>\mu_k$, (1.1) has a solution of the form*

$$u=\sum_{j=1}^k V_{x_{\mu,j},\lambda_{\mu,j}}+\omega_{\mu,k},$$

satisfying that as $\mu\to+\infty$,

(i) $x_{\mu,j}\in S$, $x_{\mu,j}\to x_j$ *with* $H(x_j)=\min_{x\in S}H(x)$, $\lambda_{\mu,j}\to+\infty$, $j=1,\cdots,k$;
(ii) $\lambda_{\mu,i}\lambda_{\mu,j}|x_{\mu,i}-x_{\mu,j}|^2\to+\infty$, $i\ne j$;

(iii) $\|\omega_{\lambda,k}\| = o(1)$.

If $x_0 \in \partial\Omega$ is a strict local minimum point of $H(x)$ with $H(x_0) > 0$, then by Theorem 1.1, (1.1) has a solution with its boundary peaks clustering near x_0. A direct consequence of Theorem 1.1 is the following.

Corollary 1.2. *Suppose that there is a connected component Γ of $\partial\Omega$ such that $H(x) > 0$ for all $x \in \Gamma$. Then, for any integer $k \geq 1$, there is an $\mu_k > 0$, depending on k, such that for any $\mu > \mu_k$,* (1.1) *has a solution of the form*

$$u = \sum_{j=1}^{k} V_{x_{\mu,j},\lambda_{\mu,j}} + \omega_{\mu,k},$$

satisfying that as $\lambda \to +\infty$,

(i) $x_{\mu,j} \in \Gamma$, $x_{\mu,j} \to x_j$ *with* $H(x_j) = \min_{x\in\Gamma} H(x)$, $\lambda_{\mu,j} \to +\infty$, $j = 1, \cdots, k$;
(ii) $\lambda_{\mu,i}\lambda_{\mu,j}|x_{\mu,i} - x_{\mu,j}|^2 \to +\infty$, $i \neq j$;
(iii) $\|\omega_{\lambda,k}\| = o(1)$.

If Ω is strictly convex, then $\min_{x\in\partial\Omega} H(x) > 0$. So, by Corollary 1.2, (1.1) has multiple boundary peak solutions. More generally, Corollary 1.2 holds if $\Omega = D \setminus \cup_{i=1}^m D_i$, where D is a strictly convex domain, and $D_i \subset\subset D$, $i = 1, \cdots, m$. Corollary 1.2 generalizes Grossi's result [15].

Theorem 1.1 has been proved by Lin, Wang and Wei [23] under more restrictive assumptions: $N \geq 7$ *and $H(P)$ has a nondegenerate local minimum.* Here we cover all $N \geq 3$ and all possible degenerate minimums.

Before we close this section, let us outline the proof of Theorem 1.1.

We first reduce the proof of Theorem 1.1 to a finite dimensional problem. To achieve this goal, for any integer $k > 0$, $\mathbf{x} = (x_1, \cdots, x_k) \in \partial\Omega \times \cdots \times \partial\Omega$, $\lambda = (\lambda_1, \cdots, \lambda_k) \in R^1_+ \times \cdots \times R^1_+$, we define

$$E_{\mathbf{x},\lambda} = \Big\{\omega :\ \omega \in H^1(\Omega), \big\langle \omega, \frac{\partial V_{x_j,\lambda_j}}{\partial \lambda_j}\big\rangle = \big\langle \omega, \frac{\partial V_{x_j,\lambda_j}}{\partial t_{j,h}}\big\rangle = 0,\\ h = 1, \cdots, N-1,\ j = 1, \cdots, k\Big\},$$

where $t_{j,h}$ forms a base of the tangent space of $\partial\Omega$ at $x_j \in \partial\Omega$. We define a set $\mathcal{M}_\mu$, which consists of points $(\mathbf{x}, \lambda)$ such that x_j lies in Γ and $\lambda_i\lambda_j|x_i - x_j|^2 \to +\infty$ for $i \neq j$. (See (2.1) in Section 2, (3.3) and (3.4) in Section 3.) We then prove that there exists a C^1 map $\omega_{\mathbf{x},\lambda}$ from $\mathcal{M}_\mu$ to $H^1(\Omega)$, such that $\omega_{\mathbf{x},\lambda} \in E_{\mathbf{x},\lambda}$, and

$$\frac{\partial J_\mu(\mathbf{x}, \lambda, \omega_{\mathbf{x},\lambda})}{\partial \omega} = \sum_{j=1}^{k} A_j \frac{\partial V_{x_j,\lambda_j}}{\partial \lambda_j} + \sum_{j=1}^{k}\sum_{h=1}^{N-1} B_{jh} \frac{\partial V_{x_j,\lambda_j}}{\partial t_{j,h}},$$

for some constants A_j and B_{jh}, where

$$J_\mu(\mathbf{x}, \lambda, \omega) = I\Big(\sum_{j=1}^{k} V_{x_j,\lambda_j} + \omega\Big).$$

To show that $\sum_{j=1}^{k} V_{x_j,\mu_j} + \omega_{\mathbf{x},\lambda}$ is actually a solution of (1.1), we need to find a $(\mathbf{x}_\mu, \lambda_\mu) \in \mathcal{M}_\mu$, such that the corresponding constants A_j and B_{jh} are all equal to zero. It is well known that if $(\mathbf{x}_\mu, \lambda_\mu) \in \mathcal{M}_\mu$ is a critical point of the function

$$K(\mathbf{x}, \lambda) =: J_\mu(\mathbf{x}, \lambda, \omega_{\mathbf{x},\lambda}), \quad (\mathbf{x}, \lambda) \in \mathcal{M}_\mu,$$

then the corresponding constants A_j and B_{jh} are all equal to zero. This procedure has been used in many problems. For subcritical case, see [10], [18], [20], [19]. For the critical exponent case, see for example [8], [28] and [31]-[33].

The new technical ingredient of this paper is the use of *gradient flows* to find critical points of reduced energy functional which are of saddle point type. The main problem is that the locations of the spikes (which are very close) and the scaling parameters are intrinsically combined. This seems to be the first paper in constructing clustered bubbles for the critical exponent problems without nondegeneracy condition and dimension restriction. Other critical problems which involve finding a saddle point for the reduced problems can be found in [39] and [40]. In particular, we mention that in [40], clustered bubbles for a slightly subcritical problem in an exterior domain were constructed when $N \geq 4$, and it was also pointed out that the same techniques could be used to study (1.1) in the case $N \geq 5$. But in [40], the existence of a critical point for the reduced finite dimensional problem is proved by comparing the homology of different level sets, so some extra assumption on an isolated local critical point of $H(x)$ is needed. In this paper, we use the min-max procedure to find a critical point of the reduced energy functional, so we are able to get rid of the unnecessary assumption in [40].

The behaviors of the solutions are different between the higher dimensional case and the lower dimensional case. So we need to treat them differently. We will prove the main result for the case $N \geq 5$ and the case $N = 3, 4$ in Section 2 and Section 3 respectively. We put the calculations of the energy for the approximate solutions in the appendices. As we will see, it is quite straight forward in the calculations of the energy for the approximate solutions in the case $N \geq 5$, while it is very technical in the case $N = 3, 4$.

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2. Proof of the main result, the case $N \geq 5$

First, we will reduce the problem of finding a k-peak solution to a finite dimension problem. We define the set $M_{\mathbf{x},\lambda}$ as follows.

Let

$$f(\bar{\lambda}) = -\frac{BH_m}{\bar{\lambda}} + \frac{B_3\mu}{\bar{\lambda}^2},$$

where $H_m = \min_{x\in S} H(x) > 0$, B and B_3 are the positive constants in Proposition A.3. Then $f(t)$ has a unique critical point

$$\bar{\lambda}_\mu = \frac{2B_3\mu}{BH_m},$$

which is also a minimum point of $f(\bar\lambda)$.

Let $\tau>0$ be a small constant. Define

$$\mathcal{V}_\mu=\Big\{\mathbf{x}=(x_1,...,x_k):|x_i-x_j|\ge\frac{1}{\mu^{1-(1+\tau)/(N-2)}},\ i\ne j,\\ x_i\in S,\text{with } H(x_i)\le H_m+\mu^{-\tau},\quad i=1,\cdots,k\Big\},$$

and

$$\mathcal{M}_\mu=\Big\{(\mathbf{x},\lambda):\mathbf{x}\in\mathcal{V}_\mu,\ \lambda_i\in\big[(1-\mu^{-\tau})\bar\lambda_\mu,(1+\mu^{-\tau})\bar\lambda_\mu\big],\ i=1,\cdots,k\Big\}. \tag{2.1}$$

For $(\mathbf{x},\lambda)\in\mathcal{M}_\mu$ and $N\ge3$, we define (as introduced in [7])

$$\varepsilon_{ij}=\frac{1}{\lambda_i^{(N-2)/2}\lambda_j^{(N-2)/2}|x_i-x_j|^{N-2}}. \tag{2.2}$$

Proposition 2.1. *There is an $\mu_k>0$, such that for each $\mu\ge\mu_k$, there exists a C^1-map $\omega_{\mathbf{x},\lambda}$: $\mathcal{M}_\mu\to H^1(\Omega)$, such that $\omega_{\mathbf{x},\lambda}\in E_{\mathbf{x},\lambda}$, and*

$$\frac{\partial J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda})}{\partial\omega}=\sum_{i=1}^k A_i\frac{\partial U_{x_i,\lambda_i}}{\partial\lambda_i}+\sum_{i=1}^k\sum_{h=1}^{N-1}B_{ih}\frac{\partial U_{x_i,\lambda_i}}{\partial t_{i,h}}, \tag{2.3}$$

for some constants A_i and B_{ih}. Moreover, we have

$$\|\omega_{\mathbf{x},\lambda}\|\le C\sum_{i\ne j}\varepsilon_{ij}^{\frac12+\sigma}+C\sum_{j=1}^k\Big(\big(\frac{\mu}{\lambda_j^2}\big)^{\frac12+\sigma}+\frac{1}{\lambda_j}\Big),$$

where $\sigma>0$ is a fixed small constant.

Proof. The proof is similar to that of [29]. We expand $J_\mu(\mathbf{x},\lambda,\omega)$ at $\omega=0$ as follows:

$$J_\mu(\mathbf{x},\lambda,\omega)=J_\mu(\mathbf{x},\lambda,0)+\big\langle l_\mu,\omega\big\rangle+\frac12\big\langle Q_\mu\omega,\omega\big\rangle+R_\mu(\omega),$$

where $l_\mu\in E_{\mathbf{x},\lambda}$ satisfying

$$\big\langle l_\mu,\omega\big\rangle=\int_\Omega\sum_{j=1}^k\nabla U_{x_j,\lambda_j}\nabla\omega+\mu\int_\Omega\sum_{j=1}^k U_{x_j,\lambda_j}\omega\\ -\int_\Omega\Big(\sum_{j=1}^k U_{x_j,\lambda_j}\Big)^{2^*-1}\omega,\quad\forall\omega\in E_{\mathbf{x},\lambda}, \tag{2.4}$$

and Q_μ is a bounded linear map from $E_{\mathbf{x},\lambda}$ to $E_{\mathbf{x},\lambda}$, satisfying

$$\begin{aligned}\langle Q_\mu \omega, \eta\rangle =& \int_\Omega \nabla\omega\nabla\eta + \mu\int_\Omega \omega\eta \\ & - (2^*-1)\int_\Omega \big(\sum_{j=1}^k U_{x_j,\lambda_j}\big)^{2^*-2}\omega\eta, \quad \omega,\ \eta\in E_{\mathbf{x},\lambda},\end{aligned} \tag{2.5}$$

and $R_\mu(\omega)$ collects all the other terms, satisfying

$$R_\mu^{(j)}(\omega) = O(\|\omega\|^{\min(2^*,3)-j}), \quad j=0,1,2.$$

Thus, to find a critical point for $J_\mu(\mathbf{x},\lambda,\omega)$ in $E_{\mathbf{x},\lambda}$ is equivalent to solving

$$l_\mu + Q_\mu\omega + R'_\mu(\omega) = 0. \tag{2.6}$$

Similar to Proposition 3.1 of [7] (see also [29]), we have

$$\|Q_\mu\omega\| \ge c'\|\omega\|, \quad \forall\, \omega\in E_{\mathbf{x},\lambda}.$$

So Q_μ is invertible in $E_{\mathbf{x},\lambda}$, and there is a constant $C>0$, such that $\|Q_\mu^{-1}\|\le C$. It follows from the implicit function theory that there is a $\omega_{\mathbf{x},\lambda}\in E_{\mathbf{x},\lambda}$, such that (2.6) holds. Moreover,

$$\|\omega_{x,\mu}\| \le C\|l_\mu\|.$$

To finish the proof of this proposition, it remains to estimate $\|l_\mu\|$. We have

$$\begin{aligned}\langle l_\mu,\omega\rangle =& \mu\int_\Omega \sum_{j=1}^k U_{x_j,\lambda_j}\omega + \sum_{j=1}^k \int_{\partial\Omega}\frac{\partial U_{x_j,\lambda_j}}{\partial n}\omega \\ & - \int_\Omega \Big(\big(\sum_{j=1}^k U_{x_j,\lambda_j}\big)^{2^*-1} - \sum_{j=1}^k U_{x_j,\lambda_j}^{2^*-1}\Big)\omega \\ =&: l_1 + l_2 + l_3.\end{aligned}$$

To estimate l_3, we use

$$\Big|\big(\sum_{j=1}^k U_{x_j,\lambda_j}\big)^{2^*-1} - \sum_{j=1}^k U_{x_j,\lambda_j}^{2^*-1}\Big| \le C\sum_{j\ne i} U_{x_j,\lambda_j}^{(2^*-1)/2}U_{x_i,\lambda_i}^{(2^*-1)/2}, \quad N\ge 6;$$

and

$$\Big|\big(\sum_{j=1}^k U_{x_j,\lambda_j}\big)^{7/3} - \sum_{j=1}^k U_{x_j,\lambda_j}^{7/3}\Big| \le C\sum_{j\ne i} U_{x_j,\lambda_j}U_{x_i,\lambda_i}^{4/3}, \quad N=5.$$

Then, by Lemma 1.2 and Estimate 3 of [7], it is easy to check that there is a small $\sigma>0$ such that

$$|l_3| \le C\sum_{i\ne j}\varepsilon_{ij}^{\frac12+\sigma}\|\omega\|.$$

On the other hand, we have

$$\begin{aligned}
&\Big|\int_{\partial\Omega}\frac{\partial U_{x_j,\lambda_j}}{\partial n}\omega\Big|\le C\int_{\partial\Omega}\frac{\lambda_j^{(N-2)/2}\lambda_j^2|y-x_j|^2}{(1+\lambda_j^2|y-x_j|^2)^{N/2}}|\omega|\\
\le& C\lambda_j^{(N-2)/2}\Big(\int_{\partial\Omega}\big(\frac{\lambda_j^2|y-x_j|^2}{(1+\lambda_j^2|y-x_j|^2)^{N/2}}\big)^{2(N-1)/N}\Big)^{N/2(N-1)}\|\omega\| \qquad (2.7)\\
\le&\frac{C}{\lambda_j}\|\omega\|.
\end{aligned}$$

Finally, take $\sigma\in(0,1)$ small, such that

$$\frac{(2^*-2)N}{2(2+(2^*-2)\sigma)}>1.$$

Let $q=2(1-\sigma)+2^*\sigma>2$. Since $N\ge5$, we can choose $\sigma>0$ small, such that $q<N/2$. Then

$$\begin{aligned}
&\Big|\mu\int_\Omega U_{x_j,\lambda_j}\omega\Big|\le\mu\big(\int_\Omega U_{x_j,\lambda_j}^{q/(q-1)}\big)^{1-1/q}|\omega|_q\\
\le& C\mu\lambda_j^{-\frac{N(q-1)}{q}+\frac{N-2}{2}}|\omega|_2^{1-\sigma}|\omega|_{2^*}^{\sigma}\le C\mu^{(1+\sigma)/2}\lambda_j^{-\frac{N(q-1)}{q}+\frac{N-2}{2}}\|\omega\|\\
=& C\mu^{(1+\sigma)/2}\lambda_j^{-1-\sigma\frac{(2^*-2)N}{2(2+(2^*-2)\sigma)}}\|\omega\|\\
\le& C\mu^{(1+\sigma)/2}\lambda_j^{-1-\sigma}\|\omega\|.
\end{aligned}$$

So, we have proved

$$\|l_\mu\|\le C\sum_{i\ne j}\varepsilon_{ij}^{\frac12+\sigma}+C\sum_{j=1}^k\Big(\big(\frac{\mu}{\lambda_j^2}\big)^{\frac12+\sigma}+\frac{1}{\lambda_j}\Big).$$

□

Remark 2.2. The estimates for $\|l_\mu\|$ in the case $N=3$ and $N=4$ are

$$\|l_\mu\|\le C\sum_{i\ne j}\varepsilon_{ij}^{\frac12+\sigma}+C\sum_{j=1}^k\frac{\sqrt{\mu}}{\sqrt{\lambda_j}},$$

and

$$\|l_\mu\|\le C\sum_{i\ne j}\varepsilon_{ij}^{\frac12+\sigma}+C\sum_{j=1}^k\frac{\sqrt{\mu\ln\lambda_j}}{\lambda_j},$$

respectively. They are not small enough so that they are negligible in the energy expansion. This is one of the main reasons that we need to modify the approximate solutions for the cases $N=3$ and $N=4$.

Let

$$K(\mathbf{x},\lambda)=J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda}),\quad (\mathbf{x},\lambda)\in\mathcal{M}_\mu,$$

where $\omega_{\mathbf{x},\lambda}$ is the map obtained in Proposition 2.1. Then, we obtain from Proposition 2.1 that

$$\begin{aligned}K(\mathbf{x},\lambda)=&J_\mu(\mathbf{x},\lambda,0)+O(\|l_\mu\|\|\omega_{\mathbf{x},\lambda}\|+\|\omega_{\mathbf{x},\lambda}\|^2)\\ =&J_\mu(\mathbf{x},\lambda,0)+O\Big(\sum_{i\neq j}\varepsilon_{ij}^{1+\sigma}+\sum_{j=1}^{k}\Big(\big(\frac{\mu}{\lambda_j^2}\big)^{1+\sigma}+\frac{1}{\lambda_j^2}\Big)\Big).\end{aligned}\tag{2.8}$$

We need the following expansions of the derivatives of $K(\mathbf{x},\lambda)$.

Lemma 2.3. *Assume* $(\mathbf{x},\lambda)\in\mathcal{M}_\mu$. *Then*

$$\frac{\partial K(\mathbf{x},\lambda)}{\partial\lambda_j}=\frac{\partial J_\mu(\mathbf{x},\lambda,0)}{\partial\lambda_j}+\sum_{l=1}^{k}\frac{1}{\lambda_l}O\Big(\sum_{i\neq m}\varepsilon_{im}^{1+\sigma}+\sum_{i=1}^{k}\Big(\big(\frac{\mu}{\lambda_i^2}\big)^{1+\sigma}+\frac{1}{\lambda_i^2}\Big)\Big).\tag{2.9}$$

Intuitively, the estimates in Lemma 2.3 can be obtained by differentiating (2.8) with respect to λ_j. We will postpone the proof of Lemma 2.3 to the end of this section. Now we are ready to prove Theorem 1.1 in the case $N\geq 5$.

Define

$$c_2=kA+\eta,$$

and

$$c_{1,\mu}=kA+kf(\bar\lambda_\mu)-\frac{1}{\bar\lambda_\mu}\mu^{-3\tau/2}.$$

where $\eta>0$ and $\tau>0$ are small constants. For any c, let $K^c=\{(\mathbf{x},\lambda):K(\mathbf{x},\lambda)<c\}$.

Consider the following flow:

$$\begin{cases}\frac{d\mathbf{x}(t)}{dt}=-\nabla_x K(\mathbf{x}(t),\lambda(t)), & t>0;\\ \frac{d\lambda(t)}{dt}=-\nabla_\lambda K(\mathbf{x}(t),\lambda(t)), & t>0;\\ (\mathbf{x}(0),\lambda(0))=(\mathbf{x}_0,\lambda_0)\in K^{c_2}.\end{cases}\tag{2.10}$$

Then

Proposition 2.4. *Suppose that* $N\geq 5$. *Then* $(\mathbf{x}(t),\lambda(t))$ *will not leave* $\mathcal{M}_\mu$ *before it reaches* $K^{c_{1,\mu}}$.

Before we prove Proposition 2.4, we prove the following lemma.

Lemma 2.5. *For any* $\mathbf{x}\in\partial\mathcal{V}_\mu$, *we have* $(\mathbf{x},\lambda)\in K^{c_{1,\mu}}$.

Proof. Since $\bar\lambda_\mu$ is the unique minimum point of $f(\bar\lambda)$, we have

$$f(\lambda_i) = f(\bar\lambda_\mu) + \frac{1}{\bar\lambda_\mu} O(\mu^{-2\tau}), \quad \forall\, \lambda_i \in [(1 - L\mu^{-\tau})\bar\lambda_\mu, (1 + L\mu^{-\tau})\bar\lambda_\mu]. \tag{2.11}$$

Note that for $(\mathbf{x}, \lambda) \in \mathcal{M}_\mu$, $\varepsilon_{ij} \le C\mu^{-(1+\tau)}$. By (2.8) and Proposition A.3, we have

$$K(\mathbf{x}, \lambda) = kA + kf(\bar\lambda_\mu) + B\sum_{j=1}^{k} \frac{H_m - H(x_j)}{\lambda_j} - B_4 \sum_{i\ne j} \varepsilon_{ij} + O\Big(\frac{1}{\mu^{1+2\tau}}\Big). \tag{2.12}$$

Suppose that there exists $i \ne j$, such that $|x_i - x_j| = \mu^{-1+(1+\tau)/(N-2)}$. Then $\varepsilon_{ij} \sim \frac{1}{\mu^{1+\tau}}$. As a result,

$$K(\mathbf{x}, \lambda) \le kA + kf(\bar\lambda_\mu) - \frac{c'}{\mu^{1+\tau}} + O\Big(\frac{1}{\mu^{1+2\tau}}\Big) < c_{1,\mu}.$$

Thus, $(\mathbf{x}, \lambda) \in K^{c_{1,\mu}}$.

Suppose that $H(x_i) = H_m + \mu^{-\tau}$ for some $i = 1, \cdots, k$. Using (2.12), we obtain

$$\begin{aligned} K(\mathbf{x}, \lambda) \le& kA + kf(\bar\lambda_\mu) + B\frac{H_m - H(x_i)}{\lambda_i} + O\Big(\frac{1}{\mu^{1+2\tau}}\Big) \\ \le& kA + kf(\bar\lambda_\mu) - \frac{c'}{\mu^{1+\tau}} + O\Big(\frac{1}{\mu^{1+2\tau}}\Big) < c_{1,\mu}. \end{aligned}$$

Thus, $(\mathbf{x}, \lambda) \in K^{c_{1,\mu}}$.

□

Proof of Proposition 2.4. Suppose that there is a $t_0 > 0$, such that $(\mathbf{x}(t_0), \lambda(t_0)) \in \partial\mathcal{M}_\mu$. We will prove that either $(\mathbf{x}(t_0), \lambda(t_0)) \in K^{c_{1,\mu}}$, or $\frac{\partial K(\mathbf{x},\lambda)}{\partial n} > 0$ at $(\mathbf{x}(t_0), \lambda(t_0))$, where n is the outward unit normal of $\partial\mathcal{M}_\mu$ at $(\mathbf{x}(t_0), \lambda(t_0))$.

If $\mathbf{x}(t_0) \in \partial\mathcal{V}_\mu$, then it follows from Lemma 2.5 that

$$(\mathbf{x}(t_0), \lambda(t_0)) \in K^{c_{1,\mu}}.$$

If $\lambda_j(t_0) = (1 + L\mu^{-\tau})\bar\lambda_\mu$ for some j, then at $(\mathbf{x}(t_0), \lambda(t_0))$, by Proposition A.4 and Lemma 2.3,

$$\frac{\partial K(\mathbf{x}, \lambda)}{\partial n} = f''(\bar\lambda_\mu) L\bar\lambda_\mu^{1-\tau} + O\Big(\frac{1}{\mu^{2+\tau}}\Big) > 0,$$

provided $L > 0$ is large.

If $\lambda_j(t_0) = (1 - L\mu^{-\tau})\mu$ for some j, then at $(\mathbf{x}(t_0), \lambda(t_0))$,

$$\frac{\partial K(\mathbf{x}, \lambda)}{\partial n} = -f''(\bar\lambda_\mu)(-L\bar\lambda_\mu^{1-\tau}) + O\Big(\frac{1}{\mu^{2+\tau}}\Big) > 0.$$

□

Proof of Theorem 1.1. We will prove that $K(\mathbf{x},\lambda)$ has a critical point in $K^{c_2}\setminus K^{c_{1,\mu}}$.

Define

$$\tilde{\mathcal{V}}_\mu=\big\{\lambda:\lambda_i\in[(1-L\mu^{-\tau})\bar\lambda_\mu,(1+L\mu^{-\tau})\bar\lambda_\mu],\ i=1,\cdots,k\big\}.$$

Then $\mathcal{M}_\mu=\mathcal{V}_\mu\times\tilde{\mathcal{V}}_\mu$.

Let Λ be the set of maps $h(\mathbf{x},\lambda)$ from $\mathcal{M}_\mu$ to $\mathcal{M}_\mu$, satisfying

$$h_1(\mathbf{x},\lambda)=\mathbf{x},\quad \text{if } (\mathbf{x},\lambda)\in\partial\mathcal{V}_\mu\times\tilde{\mathcal{V}}_\mu,$$

where $h(\mathbf{x},\lambda)=(h_1(\mathbf{x},\lambda),h_2(\mathbf{x},\lambda))$, $h_1(\mathbf{x},\lambda)\in\mathcal{V}_\mu$, $h_2(\mathbf{x},\lambda)\in\tilde{\mathcal{V}}_\mu$.

Define

$$c_\mu=\inf_{h\in\Lambda}\sup_{(\mathbf{x},\lambda)\in\mathcal{M}_\mu}K(h(\mathbf{x},\lambda)).$$

We will show that c_μ is a critical value of $K(\mathbf{x},\lambda)$. To prove this claim, we need to prove

(i) $c_{1,\mu}<c_\mu<c_2$;

(ii) $\sup_{(\mathbf{x},\lambda)\in\partial\mathcal{V}_\mu\times\tilde{\mathcal{V}}_\mu}K(h(\mathbf{x},\lambda))<c_{1,\mu}$, $\forall\, h\in\Lambda$.

To prove (ii), let $h\in\Lambda$. Then, for any $(\mathbf{x},\lambda)\in\partial\mathcal{V}_\mu\times\tilde{\mathcal{V}}_{mu}$, we have $h(\mathbf{x},\lambda)=(\mathbf{x},\tilde\lambda)$ for some $\tilde\lambda\in\tilde{\mathcal{V}}_\mu$. By Lemma 2.5, we obtain

$$K(\mathbf{x},\tilde\lambda)<c_{1,\mu}.$$

Now, we prove (i). It is easy to see $c_\mu<c_2$. For any $h\in\Lambda$, take $\tilde\lambda_i=\bar\lambda_\mu$, $i=1,\cdots,k$. Then $\bar h(\mathbf{x}):=h_1(\mathbf{x},\tilde\lambda)$ is a map from $\mathcal{V}_\mu$ to $\mathcal{V}_\mu$, satisfying

$$\bar h(\mathbf{x})=\mathbf{x},\quad\forall\,\mathbf{x}\in\partial\mathcal{V}_\mu.$$

Therefore, for any $\mathbf{z}\in\mathbf{V}_\mu$, there is a $\mathbf{x}\in\mathcal{V}_\mu$, such that $\bar h(\mathbf{x})=\mathbf{z}$. Let $\bar\lambda=h_2(\mathbf{x},\tilde\lambda)\in\tilde{\mathcal{V}}_\mu$. We have

$$\sup_{(\mathbf{x},\lambda)\in\mathcal{M}_\mu}K(h(\mathbf{x},\lambda))\ge K(\mathbf{z},\bar\lambda).$$

So, we see that we only need to choose $\mathbf{z}\in\mathcal{V}_\mu$, such that for all $\lambda\in\tilde{\mathcal{V}}_\mu$,

$$K(\mathbf{z},\lambda)\ge kA+kf(\bar\lambda_\mu)-\frac{1}{\mu^{1+2\tau}}.$$

Let $x_0\in S$ be such that $H(x_0)=H_m$. Choose $z_{\mu,j}\in B_{\mu^{-2\tau}}(x_0)$, $j=1,\cdots,k$, satisfying $|z_{\mu,i}-z_{\mu,j}|\ge c'\mu^{-2\tau}$, $\forall\, i\ne j$, where $c'>0$ is a small constant. For this $\mathbf{z}_\mu=(z_{\mu,1},\cdots,z_{\mu,k})$, we have

$$\begin{aligned}\varepsilon_{ij}=&\frac{1}{\lambda_i^{(N-2)/2}\lambda_j^{(N-2)/2}|z_{\mu,i}-z_{\mu,j}|^{N-2}}\le\frac{C}{\mu^{(N-2)(1-2\tau)}}\\=&O\Big(\frac{1}{\mu^2}\Big),\end{aligned}$$

and

$$|H(z_{\mu,i})-H_m|=O(|z_{\mu,i}-x_0|^2)=O(\mu^{-4\tau}).$$

So, from (2.12), we obtain

$$K(\mathbf{z}_\mu,\lambda)=kA+kf(\bar\lambda_\mu)+O\big(\frac{1}{\mu^{1+4\tau}}\big)>kA+kf(\bar\lambda_\mu)-\frac{1}{\mu^{1+2\tau}}. \tag{2.13}$$

□

In the rest of this section, we prove Lemma 2.3.

Proof of Lemma 2.3. Using Proposition 2.1, we find

$$\begin{aligned}\frac{\partial K(\mathbf{x},\lambda)}{\partial\lambda_i}&=\frac{\partial J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda})}{\partial\lambda_i}+\big\langle\frac{\partial J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda})}{\partial\omega},\frac{\partial\omega_{\mathbf{x},\lambda}}{\partial\lambda_i}\big\rangle\\ =&\frac{\partial J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda})}{\partial\lambda_i}+\sum_{j=1}^k A_j\big\langle\frac{\partial U_{x_j,\lambda_j}}{\partial\lambda_j},\frac{\partial\omega_{\mathbf{x},\lambda}}{\partial\lambda_i}\big\rangle+\sum_{j=1}^k\sum_{h=1}^{N-1}B_{jh}\big\langle\frac{\partial U_{x_j,\lambda_j}}{\partial t_{jh}},\frac{\partial\omega_{\mathbf{x},\lambda}}{\partial\lambda_i}\big\rangle\\ =&\frac{\partial J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda})}{\partial\lambda_i}-A_i\big\langle\frac{\partial^2 U_{x_i,\lambda_i}}{\partial\lambda_i^2},\omega_{\mathbf{x},\lambda}\big\rangle-\sum_{h=1}^{N-1}B_{ih}\big\langle\frac{\partial^2 U_{x_i,\lambda_i}}{\partial t_{ih}\partial\lambda_i},\omega_{\mathbf{x},\lambda}\big\rangle.\end{aligned} \tag{2.14}$$

Thus, to estimate $\frac{\partial K(\mathbf{x},\lambda)}{\partial\lambda_i}$, we need to estimate $\frac{\partial J_\mu(x,\mu,\omega_{\mathbf{x},\lambda})}{\partial\lambda_i}$, A_j and B_{jh}.

First, we estimate $\frac{\partial J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda})}{\partial\lambda_i}$. It is easy to check that

$$\begin{aligned}\frac{\partial J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda})}{\partial\lambda_i}&=\frac{\partial J_\mu(\mathbf{x},\lambda,0)}{\partial\lambda_i}+\sum_{j=1}^k\frac{1}{\lambda_j}O\big(\|l_\mu\|\|\omega_{\mathbf{x},\lambda}\|+\|\omega_{\mathbf{x},\lambda}\|^2\big)\\ =&\frac{\partial J_\mu(\mathbf{x},\lambda,0)}{\partial\lambda_j}+\sum_{l=1}^k\frac{1}{\lambda_l}O\Big(\sum_{i\neq m}\varepsilon_{mi}^{1+\sigma}+\sum_{i=1}^k\Big(\big(\frac{\mu}{\lambda_i^2}\big)^{1+\sigma}+\frac{1}{\lambda_i^2}\Big)\Big).\end{aligned} \tag{2.15}$$

Next, we estimate A_j and B_{jh}.
Similar to (2.15), we have

$$\begin{aligned}\frac{\partial J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda})}{\partial t_{jh}}&=\frac{\partial J_\mu(x,\mu,0)}{\partial t_{jh}}+\sum_{j=1}^k\lambda_j O\big(\|l_\mu\|\|\omega_{\mathbf{x},\lambda}\|+\|\omega_{\mathbf{x},\lambda}\|^2\big)\\ =&\frac{\partial J_\mu(\mathbf{x},\lambda,0)}{\partial t_{jh}}+\sum_{l=1}^k\lambda_l O\Big(\sum_{i\neq m}\varepsilon_{mi}^{1+\sigma}+\sum_{i=1}^k\Big(\big(\frac{\mu}{\lambda_i^2}\big)^{1+\sigma}+\frac{1}{\lambda_i^2}\Big)\Big).\end{aligned} \tag{2.16}$$

From Proposition 2.1, (2.15) and (2.16), we know that A_i and B_{ih} satisfy

$$\sum_{j=1}^{k}\langle\frac{\partial U_{x_j,\lambda_j}}{\partial\lambda_j},\frac{\partial U_{x_i,\lambda_i}}{\partial\lambda_i}\rangle A_j+\sum_{j=1}^{k}\sum_{h=1}^{N-1}\langle\frac{\partial U_{x_j,\lambda_j}}{\partial t_{jh}},\frac{\partial U_{x_i,\lambda_i}}{\partial\lambda_i}\rangle B_{jh}$$
$$=\langle\frac{\partial J_\mu}{\partial\omega},\frac{\partial U_{x_i,\lambda_i}}{\partial\lambda_i}\rangle=O\Big(\frac{1}{\mu^2}\Big); \tag{2.17}$$

$$\sum_{j=1}^{k}\langle\frac{\partial U_{x_j,\lambda_j}}{\partial\lambda_j},\frac{\partial U_{x_i,\lambda_i}}{\partial t_{im}}\rangle A_j+\sum_{j=1}^{k}\sum_{h=1}^{N-1}\langle\frac{\partial U_{x_j,\lambda_j}}{\partial t_{jh}},\frac{\partial U_{x_i,\lambda_i}}{\partial t_{im}}\rangle B_{jh}$$
$$=\langle\frac{\partial J_\mu}{\partial\omega},\frac{\partial U_{x_i,\lambda_i}}{\partial t_{im}}\rangle=O(1). \tag{2.18}$$

Noting that

$$\langle\frac{\partial U_{x_j,\lambda_j}}{\partial\lambda_j},\frac{\partial U_{x_i,\lambda_i}}{\partial\lambda_i}\rangle=\frac{\delta_{ij}}{\lambda_i^2}\big(c^*+o(1)\big),$$
$$\langle\frac{\partial U_{x_j,\lambda_j}}{\partial t_{jh}},\frac{\partial U_{x_i,\lambda_i}}{\partial\lambda_i}\rangle=o\big(\frac{1}{\lambda_i^2}+\frac{1}{\lambda_j^2}\big),$$

and

$$\langle\frac{\partial U_{x_j,\lambda_j}}{\partial t_{jh}},\frac{\partial U_{x_i,\lambda_i}}{\partial t_{im}}\rangle=\delta_{ij}\delta_{hm}\lambda_i^2\big(c^{**}+o(1)\big),$$

where c^* and c^{**} are some positive constants, we can solve (2.17) and (2.18) to obtain

$$A_j=O(1),\quad B_{jh}=O\big(\frac{1}{\mu^2}\big). \tag{2.19}$$

Combining (2.14), (2.15) and (2.19), we obtain the result.

□

3. Proof of the main result, the cases $N=3,4$

Using the estimates in Appendix B and Appendix C, we can prove Theorem 1.1 for $N=3,4$, by following the same procedure as in Section 2. Here, we just point out the differences and give the details in dealing with them.

If $N=3$, we let

$$f_3(\bar\lambda)=-\frac{BH_m}{\bar\lambda}\big(\ln\frac{\bar\lambda}{\sqrt{\mu}}+\gamma\big)+\frac{B_3\sqrt{\mu}}{\bar\lambda}.$$

Then $f_3(\bar\lambda)$ has a critical point $\bar\lambda_{3,\mu}\sim\sqrt{\mu}e^{\frac{B_3\sqrt{\mu}}{BH_m}}$. Moreover,

$$f''(\bar\lambda_{3,\mu})=\frac{2BH_m}{\bar\lambda_{3,\mu}^3}, \tag{3.1}$$

and

$$f^{(l)}(\bar\lambda_{3,\mu})=O\Big(\frac{1}{\bar\lambda_{3,\mu}^{l+1}}\Big),\quad l\ge 3. \tag{3.2}$$

Define

$$\mathcal{V}_{3,\mu}=\Big\{\mathbf{x}:|x_i-x_j|e^{\sqrt{\mu}|x_i-x_j|}\ge\mu^{\tau},\ i\ne j,\\ x_i\in S,\text{with } H(x_i)\le H_m+\mu^{-\tau},\quad i=1,\cdots,k,\Big\},$$

and

$$\mathcal{M}_{3,\mu}=\Big\{(\mathbf{x},\lambda):\mathbf{x}\in\mathcal{V}_{3,\mu},\ \lambda_i\in\big[(1-L\mu^{-\tau})\bar\lambda_{3,\mu},(1+L\mu^{-\tau})\bar\lambda_{3,\mu}\big],\ i=1,\cdots,k.\Big\} \tag{3.3}$$

If $N=4$, we let

$$f_4(\bar\lambda)=-\frac{BH_m}{\bar\lambda}+\frac{B_3\mu\ln\bar\lambda}{\bar\lambda^2}.$$

Then $f_4(\bar\lambda)$ has a critical point $\bar\lambda_{4,\mu}\sim\frac{B_3\mu\ln\mu}{BH_m}$.

Define

$$\mathcal{V}_{4,\mu}=\Big\{\mathbf{x}:\frac{|x_i-x_j|^2}{\bar K(\sqrt{\mu}|x_i-x_j|)}\ge\frac{1}{\bar\lambda_{4,\mu}}\Big(\frac{\ln\mu}{\ln\ln\mu}\Big)^{\tau},\ i\ne j,\\ x_i\in S,\text{with } H(x_i)\le H_m+\Big(\frac{\ln\ln\mu}{\ln\mu}\Big)^{\tau},\quad i=1,\cdots,k,\Big\},$$

where $\bar K(t)=tK_1(t)$, and $K_1(t)$ is a Bessel function. That is, K_1 satisfies

$$t^2K_1''+tK_1'-(t^2+1)K_1=0,\quad t>0.$$

Let

$$\mathcal{M}_{4,\mu}=\Big\{(\mathbf{x},\lambda):\mathbf{x}\in\mathcal{V}_{4,\mu},\\ \lambda_i\in\Big[\Big(1-L\Big(\frac{\ln\ln\mu}{\ln\mu}\Big)^{\tau}\Big)\bar\lambda_{4,\mu},\Big(1+L\Big(\frac{\ln\ln\mu}{\ln\mu}\Big)^{\tau}\Big)\bar\lambda_{4,\mu}\Big],\ i=1,\cdots,k.\Big\} \tag{3.4}$$

Proposition 3.1. *Let $N=3$ or 4. There is an $\mu_k>0$, such that for each $\mu\ge\mu_k$, there exists a C^1-map $\omega_{\mathbf{x},\lambda}$: $\mathcal{M}_{\mu,N}\to H^1(\Omega)$, such that $\omega_{\mathbf{x},\lambda}\in E_{\mathbf{x},\lambda}$, and*

$$\frac{\partial J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda})}{\partial\omega}=\sum_{i=1}^k A_i\frac{\partial V_{\mathbf{x},\lambda_i}}{\partial\lambda_i}+\sum_{i=1}^k\sum_{h=1}^{N-1}B_{ih}\frac{\partial V_{x_i,\lambda_i}}{\partial t_{i,h}}, \tag{3.5}$$

for some constants A_i and B_{ih}. Moreover, we have

$$\|\omega_{\mathbf{x},\lambda}\|\le C\sum_{i\ne j}\varepsilon_{ij}^{\frac12+\sigma}+C\sum_{j=1}^k\Big(\frac{\sqrt{\mu}}{\lambda_j}+\frac{1}{\mu^{1/4}\lambda_j^{1/2}}\Big),\quad \textit{if } N=3;$$

$$\|\omega_{\mathbf{x},\lambda}\| \le C\sum_{i\neq j}\varepsilon_{ij}^{\frac{1}{2}+\sigma} + C\sum_{j=1}^{k}\frac{\ln\mu}{\lambda_j}, \quad \text{if } N=4.$$

Proof. If $N=3$, $l_\mu \in E_{\mathbf{x},\lambda}$ satisfies

$$\begin{aligned}\langle l_\mu,\omega\rangle =& \sum_{j=1}^{k}\int_{\partial\Omega}\frac{\partial V_{x_j,\lambda_j}}{\partial n}\omega + \mu\sum_{j=1}^{k}\int_{\Omega}\big(U_{x_j,\lambda_j} - \frac{c_0}{\lambda_j^{1/2}|y-x_j|}\big)\omega \\ &+ \sum_{j=1}^{k}\int_{\Omega}\Big(U^5_{x_j,\lambda_j} - V^5_{x_j,\lambda_j}\Big)\omega \\ &- \int_{\Omega}\Big(\big(\sum_{j=1}^{k}V_{x_j,\lambda_j}\big)^5 - \sum_{j=1}^{k}V^5_{x_j,\lambda_j}\Big)\omega, \quad \forall\omega\in E_{\mathbf{x},\lambda}.\end{aligned} \tag{3.6}$$

By (C.51) and (C.52) in [29], we have

$$\Big(\int_{\partial\Omega}\big|\frac{\partial V_{x_j,\lambda_j}}{\partial n}\big|^{4/3}\Big)^{3/4} = O\big(\frac{1}{\lambda_j^{1/2}\mu^{1/4}}\big),$$

and

$$\Big(\int_{\Omega}\big|U_{x_j,\lambda_j} - \frac{c_0}{\lambda_j^{1/2}|y-x_j|}\big|^{6/5}\Big)^{5/6} = O\big(\frac{1}{\lambda_j^2}\big).$$

By (3.12), (3.13) and (3.14) of [29],

$$\int_{\Omega}\Big(U^5_{x_j,\lambda_j} - V^5_{x_j,\lambda_j}\Big)\omega = O\Big(\int_{\Omega}\big(U^4_{x_j,\lambda_j}|\varphi_{x_j,\lambda_j}| + |\varphi_{x_j,\lambda_j}|^5\big)|\omega| = O\big(\frac{\sqrt{\mu}}{\lambda_j}\big)\|\omega\|$$

where we denote

$$\varphi_{x_j,\lambda_j} = U_{x_j,\lambda_j} - V_{x_j,\lambda_j}. \tag{3.7}$$

So, we obtain

$$\|l_\mu\| \le C\sum_{i\neq j}\varepsilon_{ij}^{\frac{1}{2}+\sigma} + C\sum_{j=1}^{k}\Big(\frac{\sqrt{\mu}}{\lambda_j} + \frac{1}{\mu^{1/4}\lambda_j^{1/2}}\Big), \quad \text{if } N=3.$$

If $N=4$, $l_\mu\in E_{\mathbf{x},\lambda}$ satisfies

$$\begin{aligned}\langle l_\mu,\omega\rangle =& \sum_{j=1}^{k}\int_{\partial\Omega}\frac{\partial V_{x_j,\lambda_j}}{\partial n}\omega + \sum_{j=1}^{k}\int_{\Omega}\big(U^3_{x_j,\lambda_j} - V^3_{x_j,\lambda_j}\big)\omega \\ &- \int_{\Omega}\Big(\big(\sum_{j=1}^{k}V_{x_j,\lambda_j}\big)^3 - \sum_{j=1}^{k}V^3_{x_j,\lambda_j}\Big)\omega, \quad \forall\omega\in E_{\mathbf{x},\lambda}.\end{aligned} \tag{3.8}$$

Similar to (2.7), we can deduce

$$\int_{\partial\Omega}\frac{\partial V_{x_j,\lambda_j}}{\partial n}\omega = O\big(\frac{\ln\mu}{\lambda_j}\big)\|\omega\|.$$

Moreover,

$$\begin{aligned}
&\int_{\Omega}(U^3_{x_j,\lambda_j}-V^3_{x_j,\lambda_j})\omega\\
=&\int_{B_{\lambda_j^{-1/2}}(x_j)}(U^3_{x_j,\lambda_j}-V^3_{x_j,\lambda_j})\omega+\int_{\Omega\setminus B_{\lambda_j^{-1/2}}(x_j)}(U^3_{x_j,\lambda_j}-V^3_{x_j,\lambda_j})\omega\\
=&O\Big(\int_{B_{\lambda_j^{-1/2}}(x_j)}(U^2_{x_j,\lambda_j}\varphi_{x_j,\lambda_j}+\varphi^3_{x_j,\lambda_j})|\omega|+\int_{\Omega\setminus B_{\lambda_j^{-1/2}}(x_j)}U^3_{x_j,\lambda_j}|\omega|\Big)\\
=&O\Big(\big(\int_{B_{\lambda_j^{-1/2}}(x_j)}(U^{8/3}_{x_j,\lambda_j}\ln^{4/3}\lambda_j+\ln^4\lambda_j)\big)^{3/4}+\big(\int_{\Omega\setminus B_{\lambda_j^{-1/2}}(x_j)}U^4_{x_j,\lambda_j}\big)^{3/4}\Big)\|\omega\|\\
=&O\Big(\frac{\ln\lambda_j}{\lambda_j}+\frac{\ln^3\lambda_j}{\lambda_j^{3/2}}+\frac{1}{\lambda_j^{3/2}}\Big)\|\omega\|=O\big(\frac{\ln\mu}{\lambda_j}\big)\|\omega\|.
\end{aligned}$$

So,

$$\|l_\mu\|\le C\sum_{i\neq j}\varepsilon_{ij}^{\frac12+\sigma}+C\sum_{j=1}^{k}\frac{\ln\mu}{\lambda_j},\quad \text{if } N=4.$$

So, Proposition 3.1 can be proved in the same way as in Proposition 2.1. □

Let

$$K(\mathbf{x},\lambda)=J_\mu(\mathbf{x},\lambda,\omega_{\mathbf{x},\lambda}),\quad (\mathbf{x},\lambda)\in\mathcal{M}_{\mu,N},$$

where $\omega_{\mathbf{x},\lambda}$ is the map obtained in Proposition 3.1. Then, we obtain from Proposition 3.1 that

$$\begin{aligned}
K(\mathbf{x},\lambda)=&J_\mu(\mathbf{x},\lambda,0)+O\Big(\sum_{i\neq j}\varepsilon_{ij}^{1+\sigma}\Big)\\
&+\begin{cases}O\Big(\sum_{j=1}^k\big(\frac{\mu}{\lambda_j^2}+\frac{1}{\mu^{1/2}\lambda_j}\big)\Big), & \text{if } N=3;\\ O\Big(\sum_{j=1}^k\frac{\ln^2\mu}{\lambda_j^2}\Big), & \text{if } N=4.\end{cases}
\end{aligned}\tag{3.9}$$

We also have the following expansions of the derivatives of $K(\mathbf{x},\lambda)$.

$$
\begin{aligned}
\frac{\partial K(\mathbf{x},\lambda)}{\partial \lambda_j} =& \frac{\partial J_\mu(\mathbf{x},\lambda,0)}{\partial \lambda_j} + \frac{1}{\lambda_j} O\Big(\sum_{i\neq l} \varepsilon_{il}^{1+\sigma}\Big) \\
&+ \frac{1}{\lambda_j} \begin{cases} O\Big(\sum_{j=1}^k \big(\frac{\mu}{\lambda_j^2} + \frac{1}{\mu^{1/2}\lambda_j}\big)\Big), & \text{if } N=3; \\ O\Big(\sum_{j=1}^k \big(\frac{\ln^2\mu}{\lambda_j^2}\Big), & \text{if } N=4. \end{cases}
\end{aligned}
\tag{3.10}
$$

Define

$$c_2 = kA + \eta,$$

$$c_{1,\mu,3} = kA + kf_3(\bar{\lambda}_{\mu,3}) - \frac{1}{\mu^{3\tau/2}\bar{\lambda}_{3,\mu}},$$

and

$$c_{1,\mu,4} = kA + kf_4(\bar{\lambda}_{4,\mu}) - \frac{1}{\bar{\lambda}_{4,\mu}}\big(\frac{\ln\ln\mu}{\ln\mu}\big)^{3\tau/2},$$

where $\eta > 0$ and $\tau > 0$ are small constants.

Lemma 3.2. *For any* $\mathbf{x} \in \partial\mathcal{V}_{N,\mu}$, *we have* $(\mathbf{x},\lambda) \in K^{c_{1,\mu,N}}$.

Proof. We only prove the case $N = 3$. The case $N = 4$ can be proved in a similar way.

Using $f'(\bar{\lambda}_{3,\mu}) = 0$, (3.1) and (3.2), we obtain

$$f_3(\lambda_j) = f_3(\bar{\lambda}_{3,\mu}) + O\Big(\frac{1}{\mu^{2\tau}\bar{\lambda}_{3,\mu}}\Big) \tag{3.11}$$

Note that for $(\mathbf{x},\lambda) \in \mathcal{M}_{3,\mu}$, $e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij} \le \frac{C}{\mu^\tau\lambda_j}$. By (3.9), (3.11) and Proposition B.3, we have

$$
\begin{aligned}
K(\mathbf{x},\lambda) =& kA + kf_3(\bar{\lambda}_{3,\mu}) + B\sum_{j=1}^k \frac{H_m - H(x_j)}{\lambda_j}\big(\ln\frac{\lambda_j}{\sqrt{\mu}} + \gamma\big) \\
&- B_4\sum_{i\neq j} e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij} + O\Big(\frac{1}{\mu^{2\tau}\bar{\lambda}_{3,\mu}}\Big).
\end{aligned}
\tag{3.12}
$$

From (3.12), we can prove that if $|x_i - x_j|e^{\sqrt{\mu}|x_i-x_j|} = \mu^\tau$, for some $i \neq j$, or $H(x_i) = H_m + \mu^{-\tau}$ for some $i = 1,\cdots,k$, then $(\mathbf{x},\lambda) \in K^{c_{1,\mu}}$.

□

Proposition 3.3. *The flow* $(\mathbf{x}(t),\lambda(t))$ *will not leave* $\mathcal{M}_{N,\mu}$ *before it reaches* $K^{c_{1,\mu,N}}$.

Proof. We only prove the case $N = 3$. The case $N = 4$ can be proved in a similar way.

If $\lambda_j(t_0) = \bar{\lambda}_{3,\mu}(1 + L\mu^{-\tau})$ for some j, then

$$\frac{\partial K(\mathbf{x},\lambda)}{\partial n} = \frac{BH_m}{\bar{\lambda}_{3,\mu}^3} L\bar{\lambda}_\mu\mu^{-\tau} + O\Big(\frac{1}{\mu^\tau\bar{\lambda}_{3,\mu}^2}\Big) > 0,$$

provided $L>0$ is large.

If $\lambda_j(t_0)=\bar\lambda_{3,\mu}(1-L\mu^{-\tau})$ for some j, then

$$\frac{\partial K(\mathbf{x},\lambda)}{\partial n}=-\frac{BH_m}{\bar\lambda_{3,\mu}^2}(-L\mu^{-\tau})+O\Big(\frac{1}{\mu^\tau\bar\lambda_{3,\mu}^2}\Big)>0.$$

□

Proof of Theorem 1.1 . Suppose that $N=3$. Let $x_0\in S$ be such that $H(x_0)=H_m$. Choose $z_{\mu,j}\in B_{\mu^{-1/3}}(x_0)$, $j=1,\cdots,k$, satisfying $|z_{\mu,i}-z_{\mu,j}|\ge c'\mu^{-1/3}$, $\forall\ i\ne j$, where $c'>0$ is a small constant. For this $\mathbf{z}_\mu=(z_{\mu,1},\cdots,z_{\mu,k})$, we have

$$\frac{e^{-\sqrt{\mu}|z_{\mu,i}-z_{\mu,j}|}}{\lambda_i^{1/2}\lambda_j^{1/2}|z_{\mu,i}-z_{\mu,j}|}\le\frac{C}{\bar\lambda_{3,\mu}}e^{-\mu^{1/6}}\mu^{1/3}=O\big(\frac{1}{\mu^{2\tau}\bar\lambda_{3,\mu}}\big),$$

and

$$|H(z_{\mu,i})-H_m|=O(|z_{\mu,i}-x_0|^2)=O(\mu^{-2/3}).$$

So,

$$\frac{H(z_{\mu,j})-H_m}{\lambda_j}\big(\ln\frac{\lambda_j}{\sqrt{\mu}}+\gamma\big)=O\big(\frac{\mu^{-2/3}}{\lambda_j}\sqrt{\mu}\big)=O\big(\frac{\mu^{-1/6}}{\lambda_j}\big).$$

As a result, by (3.12),

$$K(\mathbf{z}_\mu,\lambda)=kA+kf(\bar\lambda_{3,\mu})+O\big(\frac{1}{\mu^{2\tau}\bar\lambda_{3,\mu}}\big)>kA+kf(\bar\lambda_\mu)-\frac{1}{\mu^{3\tau/2}\bar\lambda_{3,\mu}}.\tag{3.13}$$

The case $N=4$ can be treated in a similar way. □

Appendix A. Energy expansion, the case $N\ge 5$

In this section, we will expand $I(U_{x_j,\lambda_j})$ and its derivatives. Recall that $H(y)$ is the mean curvature of $\partial\Omega$ at $y\in\partial\Omega$. Direct calculations show

$$\begin{aligned}&\int_\Omega U_{x_j,\lambda_j}^{2^*}=\int_{\mathbb{R}^N}U^{2^*}-\frac{2H(x_j)}{(N-1)\lambda_j}\int_{\mathbb{R}^{N-1}}\frac{|y'|^2}{(1+|y'|^2)^N}\,dy'+O\big(\frac{1}{\lambda_j^2}\big)\\&=\int_{\mathbb{R}^N}U^{2^*}-\frac{B_1H(x_j)}{\lambda_j}+O\big(\frac{1}{\lambda_j^2}\big),\end{aligned}$$

$$\begin{aligned}&\int_\Omega|\nabla U_{x_j,\lambda_j}|^2=\int_\Omega U_{x_j,\lambda_j}^{2^*}+\int_{\partial\Omega}\frac{\partial U_{x_j,\lambda_j}}{\partial n}U_{x_j,\lambda_j}\\&=\int_{\mathbb{R}^N}U^{2^*}-\frac{B_2H(x_j)}{\lambda_j}+O\big(\frac{1}{\lambda_j^2}\big),\end{aligned}$$

and

$$\int_\Omega U_{x_j,\lambda_j}^2 = \frac{1}{\lambda_j^2}\int_{\mathbb{R}^N} U^2 + O\big(\frac{1}{\lambda_j^3}\big) = \frac{B_3}{\lambda_j^2} + O\big(\frac{1}{\lambda_j^3}\big),$$

where B_i, $i = 1, 2, 3$, is some positive constant. So we have

Proposition A.1. *Suppose that $N \geq 5$. We have the following estimate:*

$$I(U_{x_j,\lambda_j}) = A + \frac{\mu B_3}{\lambda_j^2} - \frac{BH(x_j)}{\lambda_j} + O\big(\frac{1}{\lambda_j^2}\big),$$

where $A = \frac{1}{N}\int_{\mathbb{R}^N} U^{2^*}$, B and B_3 are positive constants.

Next, we calculate

$$\begin{aligned}
&I\big(\sum_{j=1}^k U_{x_j,\lambda_j}\big)\\
=&\sum_{j=1}^k I\big(U_{x_j,\lambda_j}\big) + \sum_{i>j}\mu\int_\Omega U_{x_i,\lambda_i}U_{x_j,\lambda_j} + \sum_{i>j}\int_{\partial\Omega}\frac{\partial U_{x_i,\lambda_i}}{\partial n}U_{x_j,\lambda_j}\\
&-\frac{1}{2}\sum_{i\neq j}\int_\Omega U_{x_i,\lambda_i}^{2^*-1}U_{x_j,\lambda_j}\\
&-\frac{1}{2^*}\int_\Omega\Big(\big(\sum_{j=1}^k U_{x_j,\lambda_j}\big)^{2^*} - \sum_{j=1}^k U_{x_j,\lambda_j}^{2^*} - 2^*\sum_{i\neq j}U_{x_i,\lambda_i}^{2^*-1}U_{x_j,\lambda_j}\Big).
\end{aligned}\tag{A.1}$$

Then,

$$\frac{1}{2}\int_\Omega U_{x_i,\lambda_i}^{2^*-1}U_{x_j,\lambda_j} = B_4\varepsilon_{ij} + O\big(\varepsilon_{ij}^{1+\sigma}\big),$$

and

$$\int_\Omega\Big(\big(\sum_{j=1}^k U_{x_j,\lambda_j}\big)^{2^*} - \sum_{j=1}^k U_{x_j,\lambda_j}^{2^*} - 2^*\sum_{i\neq j}U_{x_i,\lambda_i}^{2^*-1}U_{x_j,\lambda_j}\Big) = O\Big(\sum_{i\neq j}\varepsilon_{ij}^{1+\sigma}\Big),$$

where ε_{ij} is defined at (2.2), $B_4 = \frac{1}{2}\int_{\mathbb{R}^N} U^{2^*-1} > 0$, and $\sigma > 0$ is a fixed small constant. So, (A.1) can be rewritten as

$$\begin{aligned}
I\big(\sum_{j=1}^k U_{x_j,\lambda_j}\big) =&\sum_{j=1}^k I\big(U_{x_j,\lambda_j}\big) - B_4\sum_{i\neq j}\varepsilon_{ij}\\
&+\sum_{i>j}\mu\int_\Omega U_{x_i,\lambda_i}U_{x_j,\lambda_j} + \sum_{i>j}\int_{\partial\Omega}\frac{\partial U_{x_i,\lambda_i}}{\partial n}U_{x_j,\lambda_j} + O\Big(\sum_{i\neq j}\varepsilon_{ij}^{1+\sigma}\Big).
\end{aligned}\tag{A.2}$$

Now, we estimate the two interaction terms in (A.2).

Lemma A.2. *For any small $i \neq j$,*

$$\int_\Omega U_{x_i,\lambda_i} U_{x_j,\lambda_j} = O\big(\varepsilon_{ij} |x_i - x_j|^2 \big|\ln |x_i - x_j|\big|\big),$$

and

$$\int_{\partial\Omega} \frac{\partial U_{x_i,\lambda_i}}{\partial n} U_{x_j,\lambda_j} = O\big(\varepsilon_{ij} |x_i - x_j| \big|\ln |x_i - x_j|\big|\big).$$

Proof. We have

$$\begin{aligned}
&\int_\Omega U_{x_i,\lambda_i} U_{x_j,\lambda_j} \le \frac{C}{\lambda_i^{(N-2)/2}\lambda_j^{(N-2)/2}} \int_\Omega \frac{1}{|y-x_i|^{N-2}|y-x_j|^{N-2}}\, dy \\
=& \frac{C}{\lambda_i^{(N-2)/2}\lambda_j^{(N-2)/2}} \Big(\int_{B_{\frac12|x_i-x_j|}(x_i)} + \int_{B_{\frac12|x_i-x_j|}(x_j)} \Big) \frac{1}{|y-x_i|^{N-2}|y-x_j|^{N-2}}\, dy \\
&+ \frac{C}{\lambda_i^{(N-2)/2}\lambda_j^{(N-2)/2}} \int_{\Omega \setminus \big(B_{\frac12|x_i-x_j|}(x_i) \cup B_{\frac12|x_i-x_j|}(x_j)\big)} \frac{1}{|y-x_i|^{N-2}|y-x_j|^{N-2}}\, dy \\
\le& C\varepsilon_{ij} \Big(\int_{B_{\frac12|x_i-x_j|}(x_i)} \frac{1}{|y-x_i|^{N-2}}\, dy + \int_{B_{\frac12|x_i-x_j|}(x_j)} \frac{1}{|y-x_j|^{N-2}}\, dy \Big) \\
&+ C\varepsilon_{ij} |x_i - x_j|^2 \int_{\Omega \setminus \big(B_{\frac12|x_i-x_j|}(x_i) \cup B_{\frac12|x_i-x_j|}(x_j)\big)} \frac{1}{|y-x_i|^{N/2}|y-x_j|^{N/2}}\, dy \\
\le& C\varepsilon_{ij} |x_i - x_j|^2 + C\varepsilon_{ij} |x_i - x_j|^2 \big|\ln |x_i - x_j|\big| \\
=& O\big(\varepsilon_{ij} |x_i - x_j|^2 \big|\ln |x_i - x_j|\big|\big).
\end{aligned}$$

Similarly,

$$\begin{aligned}
&\Big| \int_{\partial\Omega} \frac{\partial U_{x_i,\lambda_i}}{\partial n} U_{x_j,\lambda_j} \Big| \le C \int_{\partial\Omega} |U'_{x_i,\lambda_i}| |y - x_i| U_{x_j,\lambda_j} \\
\le& C \int_{\partial\Omega} \frac{\lambda_i^{(N-2)/2} \lambda_i^2 |y-x_i|^2}{(1+\lambda_i^2|y-x_i|^2)^{N/2}} \frac{\lambda_j^{(N-2)/2}}{(1+\lambda_j^2|y-x_j|^2)^{(N-2)/2}} \\
\le& \frac{C}{\lambda_i^{(N-2)/2}\lambda_j^{(N-2)/2}} \int_{\partial\Omega} \frac{1}{|y-x_i|^{N-2}|y-x_j|^{N-2}}\, dy \\
=& O\big(\varepsilon_{ij} |x_i - x_j| \big|\ln |x_i - x_j|\big|\big).
\end{aligned}$$

□

Combining Proposition A.1, (A.2) and Lemma A.2, we obtain

Proposition A.3. *Suppose that $N \ge 5$, $\lambda_i \sim \frac{2B_3\mu}{BH_m}$ and $|x_i - x_j| \ge \mu^{-T}$ for some large $T > 0$. We have the following estimates:*

$$
\begin{aligned}
I\Big(\sum_{j=1}^{k} U_{x_j,\lambda_j}\Big) =& kA + \sum_{j=1}^{k} \frac{\mu B_3}{\lambda_j^2} - \sum_{j=1}^{k} \frac{BH(x_j)}{\lambda_j} - B_4 \sum_{i\neq j} \varepsilon_{ij} \\
&+ O\Big(\sum_{i\neq j} \varepsilon_{ij}^{1+\sigma} + \frac{1}{\mu^{1+\sigma}}\Big),
\end{aligned}
$$

where $\sigma > 0$ is a fixed small constant.

Proof. It follows from Lemma A.2 that

$$
\begin{aligned}
I\Big(\sum_{j=1}^{k} U_{x_j,\lambda_j}\Big) =& kA + \sum_{j=1}^{k} \frac{\mu B_3}{\lambda_j^2} - \sum_{j=1}^{k} \frac{BH(x_j)}{\lambda_j} - B_4 \sum_{i> j} \varepsilon_{ij} \\
&+ O\Big(\sum_{i\neq j} \big(\mu |x_i - x_j|^2 \big|\ln |x_i - x_j|\big| \varepsilon_{ij} + |x_i - x_j| \big|\ln |x_i - x_j|\big| \varepsilon_{ij} + \varepsilon_{ij}^{1+\sigma}\big)\Big).
\end{aligned}
$$

So, to prove this proposition, we only need to show

$$
\mu |x_i - x_j|^2 \big|\ln |x_i - x_j|\big| \varepsilon_{ij} = O\Big(\frac{1}{\mu^{1+\sigma}} + \varepsilon_{ij}^{1+\sigma}\Big), \tag{A.3}
$$

and

$$
|x_i - x_j| \big|\ln |x_i - x_j|\big| \varepsilon_{ij} = O\Big(\frac{1}{\mu^{1+\sigma}} + \varepsilon_{ij}^{1+\sigma}\Big). \tag{A.4}
$$

If $|x_i - x_j| \leq \mu^{-2/3}$, then

$$
\mu |x_i - x_j|^2 \big|\ln |x_i - x_j|\big|\ \varepsilon_{ij} \leq C \mu^{-1/3} \ln \mu\ \varepsilon_{ij} = O\Big(\frac{1}{\mu^{1+\sigma}} + \varepsilon_{ij}^{1+\sigma}\Big).
$$

If $|x_i - x_j| \geq \mu^{-2/3}$, then

$$
\begin{aligned}
&\mu |x_i - x_j|^2 \big|\ln |x_i - x_j|\big|\ \varepsilon_{ij} \leq \frac{C}{\mu} \frac{\ln \mu}{\mu^{N-4} |x_i - x_j|^{N-4}} \\
\leq& \frac{C}{\mu} \frac{\ln \mu}{\mu^{(N-4)/3}} = O\Big(\frac{1}{\mu^{1+\sigma}}\Big).
\end{aligned}
$$

So, we have proved (A.3). We can prove (A.4) in a similar way. □

Before we close this section, we give the following expansions for the derivatives of $I\big(\sum_{j=1}^{k} U_{x_j,\lambda_j}\big)$.

Proposition A.4. *Suppose that $N \geq 5$, $\lambda_i \sim \frac{2B_3\mu}{BH_m}$ and $|x_i - x_j| \geq \mu^{-T}$ for some large $T > 0$. We have the following estimates:*

$$\frac{\partial}{\partial\lambda_i}I\big(\sum_{j=1}^{k}U_{x_j,\lambda_j}\big)=-\frac{2\mu B_3}{\lambda_i^3}+\frac{BH(x_i)}{\lambda_i^2}+\frac{1}{\mu}O\Big(\sum_{i\neq j}\varepsilon_{ij}+\frac{1}{\mu^{1+\sigma}}\Big),$$

and

$$\frac{\partial}{\partial x_{ih}}I\big(\sum_{j=1}^{k}U_{x_j,\lambda_j}\big)=\mu O\Big(\sum_{i\neq j}\varepsilon_{ij}+\frac{1}{\mu}\Big),$$

where $\sigma>0$ is a fixed small constant.

Proof. Using

$$\Big|\frac{\partial U_{x_i,\lambda_i}}{\partial\lambda_i}\Big|\le C\lambda_i^{-1}U_{x_i,\lambda_i},$$

and

$$\Big|\frac{\partial U_{x_i,\lambda_i}}{\partial x_{ih}}\Big|\le C\lambda_i U_{x_i,\lambda_i},$$

we can prove this proposition in a similar way as in Proposition A.3. □

Appendix B. Energy expansion, the case $N=3$

Since $N=3$, we have $c_0=3^{1/4}$. Let

$$V_{x_j,\lambda_j}=U_{x_j,\lambda_j}-\varphi_{x_j,\lambda_j},$$

where

$$\varphi_{x_j,\lambda_j}(y)=\frac{c_0}{\lambda_j^{1/2}|y-x_j|}\big(1-e^{-\sqrt{\mu}|y-x_j|}\big).$$

Then, V_{x_j,λ_j} satisfies

$$-\Delta V_{x_j,\lambda_j}+\mu V_{x_j,\lambda_j}=U_{x_j,\lambda_j}^5+\mu\Big(U_{x_j,\lambda_j}-\frac{c_0}{\lambda_j^{1/2}|y-x_j|}\Big).\tag{B.1}$$

In this section, we will expand $I(V_{x_j,\lambda_j})$ and its derivatives. By (C.3), (C.1) and (C.2) in [29],

$$\int_\Omega V_{x_j,\lambda_j}^6=\sqrt{3}\Big(\frac{3\pi^2}{8}-\frac{12\pi\sqrt{\mu}}{\lambda_j}-\frac{3\pi H(x_j)}{\lambda_j}+O\big(\frac{\mu}{\lambda_j^2}\big)\Big),$$

$$\int_\Omega|\nabla Vx_j,\lambda_j|^2=\sqrt{3}\Big(\frac{3\pi^2}{8}-\frac{3\pi\sqrt{\mu}}{\lambda_j}-\frac{\pi H(x_j)}{\lambda_j}\big(\ln\frac{\lambda_j}{\sqrt{\mu}}+\beta\big)+O\big(\frac{1}{\lambda_j\sqrt{\mu}}\big)\Big),$$

where β is a constant, and

$$\int_\Omega V_{x_j,\lambda_j}^2 = \sqrt{3}\Big(\frac{\pi}{\sqrt{\mu}\lambda_j} - \frac{\pi H(x_j)}{4\mu\lambda_j} + O\big(\frac{1}{\lambda_j\mu^{3/2}}\big)\Big).$$

So we have

Proposition B.1. *Suppose that $N=3$. We have the following estimate:*

$$I(V_{x_j,\lambda_j}) = A + \frac{B_3\sqrt{\mu}}{\lambda_j} - \frac{BH(x_j)}{\lambda_j}\big(\ln\frac{\lambda_j}{\sqrt{\mu}} + \gamma\big) + O\big(\frac{1}{\sqrt{\mu}\lambda_j} + \frac{\mu}{\lambda_j^2}\big),$$

where $A>0$, γ, $B_3>0$ and $B>0$ are constants.

Next, we calculate

$$\begin{aligned}
&I\big(\sum_{j=1}^k V_{x_j,\lambda_j}\big)\\
=&\sum_{j=1}^k I\big(V_{x_j,\lambda_j}\big) + \sum_{i>j}\int_{\partial\Omega}\frac{\partial V_{x_i,\lambda_i}}{\partial n}V_{x_j,\lambda_j}\\
&+\sum_{i>j}\mu\int_\Omega\Big(U_{x_i,\lambda_i} - \frac{c_0}{\lambda_i^{1/2}|y-x_i|}\Big)V_{x_j,\lambda_j}\\
&-\frac{1}{2}\sum_{i\neq j}\int_\Omega U_{x_i,\lambda_i}^5 V_{x_j,\lambda_j} + \sum_{i\neq j}\int_\Omega\big(U_{x_i,\lambda_i}^5 - V_{x_i,\lambda_i}^5\big)V_{x_j,\lambda_j}\\
&-\frac{1}{6}\int_\Omega\Big(\big(\sum_{j=1}^k V_{x_j,\lambda_j}\big)^6 - \sum_{j=1}^k V_{x_j,\lambda_j}^6 - 6\sum_{i\neq j}V_{x_i,\lambda_i}^{2^*-1}V_{x_j,\lambda_j}\Big).
\end{aligned} \tag{B.2}$$

Since

$$\begin{aligned}
&V_{x_j,\lambda_j} = U_{x_j,\lambda_j} - \varphi_{x_j,\lambda_j}\\
=&\frac{c_0}{\lambda_j^{1/2}}\frac{1}{|y-x_j|}e^{-\sqrt{\mu}|y-x_j|} + O\Big(\frac{1}{\lambda_j^{5/2}|x_i-x_j|^3}\Big), \quad y\in\Omega\setminus B_{\frac{1}{2}|x_i-x_j|}(x_j)
\end{aligned}$$

it is easy to check

$$\begin{aligned}
&\int_\Omega\Big(\big(\sum_{j=1}^k V_{x_j,\lambda_j}\big)^6 - \sum_{j=1}^k V_{x_j,\lambda_j}^6 - 6\sum_{i\neq j}V_{x_i,\lambda_i}^5 V_{x_j,\lambda_j}\Big)\\
=&O\Big(\int_\Omega\sum_{j\neq i}|V_{x_i,\lambda_i}|^4|V_{x_j,\lambda_j}|^2\Big) = O\Big(\sum_{i\neq j}\varepsilon_{ij}^{1+\sigma}\Big),
\end{aligned}$$

and for $i\neq j$,

$$
\begin{aligned}
&\int_\Omega U^5_{x_i,\lambda_i}V_{x_j,\lambda_j}=\int_{B_{\frac12|x_i-x_j|}(x_i)}U^5_{x_i,\lambda_i}V_{x_j,\lambda_j}+O\Big(\frac{\varepsilon_{ij}}{\lambda_i^2|x_i-x_j|^2}\Big)\\
=&2B_4\varepsilon_{ij}e^{-\sqrt{\mu}|x_i-x_j|}+O\Big(\frac{\varepsilon_{ij}}{\lambda_i^2|x_i-x_j|^2}\Big),
\end{aligned}
\tag{B.3}
$$

where $B_4>0$ is a constant.

On the other hand,

$$
\begin{aligned}
&\Big|\int_\Omega(U^5_{x_i,\lambda_i}-V^5_{x_i,\lambda_i})V_{x_j,\lambda_j}\Big|\le C\Big|\int_\Omega U^4_{x_i,\lambda_i}\varphi_{x_i,\lambda_i}V_{x_j,\lambda_j}\Big|\\
\le& C\Big|\int_{B_{\frac12|x_i-x_j|}(x_i)}U^4_{x_i,\lambda_i}\varphi_{x_i,\lambda_i}V_{x_j,\lambda_j}\Big|+O\Big(\frac{\varepsilon_{ij}}{\lambda_j^2|x_i-x_j|^2}\Big)\\
=&O\Big(\frac{1}{\lambda_j^{1/2}|x_i-x_j|}\int_{B_{\frac12|x_i-x_j|}(x_i)}U^4_{x_i,\lambda_i}\varphi_{x_i,\lambda_i}+\frac{\varepsilon_{ij}}{\lambda_j^2|x_i-x_j|^2}\Big)\\
=&O\Big(\varepsilon_{ij}\int_{B_{\frac12|x_i-x_j|\lambda_i}(0)}U^4\frac{1}{|z|}(1-e^{-\sqrt{\mu}|z|/\lambda_i})+\frac{\varepsilon_{ij}}{\lambda_j^2|x_i-x_j|^2}\Big)\\
=&\varepsilon_{ij}O\Big(\frac{\sqrt{\mu}}{\lambda_i}+\frac{1}{\lambda_j^2|x_i-x_j|^2}\Big).
\end{aligned}
\tag{B.4}
$$

So, (A.1) can be rewritten as

$$
\begin{aligned}
I\big(\sum_{j=1}^k V_{x_j,\lambda_j}\big)=&\sum_{j=1}^k I\big(V_{x_j,\lambda_j}\big)-B_4\sum_{i\ne j}e^{-\mu|x_i-x_j|}\varepsilon_{ij}\\
&+\sum_{i>j}\int_{\partial\Omega}\frac{\partial V_{x_i,\lambda_i}}{\partial n}V_{x_j,\lambda_j}+\sum_{i>j}\mu\int_\Omega\Big(U_{x_i,\lambda_i}-\frac{c_0}{\lambda_i^{1/2}|y-x_i|}\Big)V_{x_j,\lambda_j}\\
&+\varepsilon_{ij}O\Big(\sum_{i=1}^k\frac{\sqrt{\mu}}{\lambda_i}+\sum_{i\ne j}\big(\frac{1}{\lambda_j^2|x_i-x_j|^2}+\varepsilon_{ij}^\sigma\big)\Big).
\end{aligned}
\tag{B.5}
$$

Now, we estimate the two interaction terms in (B.5).

Lemma B.2. *Suppose that* $\lambda_i\sim\sqrt{\mu}e^{\frac{\bar B_1\sqrt{\mu}}{BH_m}}$ *and* $|x_i-x_j|\ge\mu^{-T}$ *for some* $T>0$ *large. For any* $i\ne j$,

$$
\int_\Omega\Big(U_{x_i,\lambda_i}-\frac{c_0}{\lambda_i^{1/2}|y-x_i|}\Big)V_{x_j,\lambda_j}=O\Big(\frac{1}{\lambda_i^2}+\frac{1}{\lambda_i\mu^4}\Big),
$$

and

$$\int_{\partial\Omega}\frac{\partial V_{x_i,\lambda_i}}{\partial n}V_{x_j,\lambda_j}=O\Big(\frac{1}{\lambda_i^2}+\mu^{-1/4}e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij}+\varepsilon_{ij}^{1+\sigma}\Big).$$

Proof. For $y\in\Omega\setminus B_{\mu^{-2}|x_i-x_j|}(x_i)$, we have

$$\lambda_i|y-x_i|\ge\lambda_i\mu^{-2}|x_i-x_j|\ge\lambda_i\mu^{-(T+2)}\to+\infty,$$

as $\mu\to+\infty$. So,

$$\begin{aligned}&\int_\Omega\Big(U_{x_i,\lambda_i}-\frac{c_0}{\lambda_i^{1/2}|y-x_i|}\Big)V_{x_j,\lambda_j}\\ \le&\frac{C\mu^6}{\lambda_i^{5/2}|x_i-x_j|^3\lambda_j^{1/2}}\int_{\Omega\setminus B_{\mu^{-2}|x_i-x_j|}(x_i)}\frac{1}{|y-x_j|}\,dy\\ &+C\Big(\frac{1}{\lambda_i^{1/2}|x_i-x_j|^3\lambda_j^{5/2}}+\frac{e^{-\sqrt{\mu}|x_i-x_j|}}{\lambda_i^{1/2}\lambda_j^{1/2}|x_i-x_j|}\Big)\int_{B_{\mu^{-2}|x_i-x_j|}(x_i)}\frac{1}{|y-x_i|}\,dy\\ =&O\Big(\frac{\mu^{6+3T}}{\lambda_i^3}\Big)+O\Big(\frac{\mu^{T-4}}{\lambda_i^3}+\frac{|x_i-x_j|e^{-\sqrt{\mu}|x_i-x_j|}}{\lambda_i\mu^4}\Big)=O\Big(\frac{1}{\lambda_i^2}+\frac{1}{\lambda_i\mu^4}\Big).\end{aligned}$$

Similar to Lemma A.2,

$$\begin{aligned}\Big|\int_{\partial\Omega}\frac{\partial V_{x_i,\lambda_i}}{\partial n}V_{x_j,\lambda_j}\Big|\le& C\int_{\partial\Omega}|V'_{x_i,\lambda_i}||y-x_i|V_{x_j,\lambda_j}\\ =&O\Big(\frac{1}{\lambda_i^2|x_i-x_j|^2}+e^{-\sqrt{\mu}|x_i-x_j|}\Big)|x_i-x_j|\,\big|\ln|x_i-x_j|\big|\,\varepsilon_{ij}\\ =&O\Big(\frac{1}{\lambda_i^2}+\mu^{-1/4}e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij}+\varepsilon_{ij}^{1+\sigma}\Big).\end{aligned}$$

□

Combining Proposition B.1, (B.2) and Lemma B.2, we obtain

Proposition B.3. *Suppose that $N=3$, $\lambda_i\sim\sqrt{\mu}e^{\frac{\bar B_1\sqrt{\mu}}{BH_m}}$ and $|x_i-x_j|\ge\mu^{-T}$ for some $T>0$ large. We have the following estimates:*

$$\begin{aligned}I\Big(\sum_{j=1}^k V_{x_j,\lambda_j}\Big)=&kA+\sum_{j=1}^k\frac{B_3\sqrt{\mu}}{\lambda_j}-\sum_{j=1}^k\frac{BH(x_j)}{\lambda_j}\Big(\ln\frac{\lambda_j}{\sqrt{\mu}}+\gamma\Big)-B_4\sum_{i\ne j}e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij}\\ &+O\Big(\sum_{i\ne j}\big(\varepsilon_{ij}^{\bar\sigma}+\frac{1}{\mu^{1/4}}\big)e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij}+\sum_{j=1}^k\frac{1}{\lambda_j\sqrt{\mu}}\Big),\end{aligned}$$

where $\bar\sigma>0$ is a fixed small constant.

Proof. It follows from Lemma B.2 that

$$I\Big(\sum_{j=1}^k V_{x_j,\lambda_j}\Big) = kA + \sum_{j=1}^k \frac{B_3\sqrt{\mu}}{\lambda_j} - \sum_{j=1}^k \frac{BH(x_j)}{\lambda_j}\Big(\ln\frac{\lambda_j}{\sqrt{\mu}} + \gamma\Big) - B_4 \sum_{i\neq j} e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij}$$
$$+ O\Big(\sum_{i\neq j}\big(\varepsilon_{ij}^{1+\sigma} + \frac{1}{\mu^{1/4}} e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij}\big) + \sum_{j=1}^k \frac{1}{\lambda_j\sqrt{\mu}}\Big).$$

To prove this proposition, we only need to show

$$\varepsilon_{ij}^{1+\sigma} = O\Big(\frac{1}{\lambda_j^{1+\bar\sigma}} + e^{-(1+\bar\sigma)\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij}^{1+\bar\sigma}\Big),$$

for some small $\bar\sigma > 0$. In fact, if $|x_i - x_j| \ge \lambda_j^{-\alpha}$, where $\alpha > 0$ is a small constant, then

$$\varepsilon_{ij}^{1+\sigma} \le \frac{C}{\lambda_j^{(1-\alpha)(1+\sigma)}} \le \frac{C}{\lambda_j^{1+\bar\sigma}}$$

If $|x_i - x_j| \le \lambda_j^{-\alpha}$, then

$$e^{(1+\sigma)\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij}^{1+\sigma} = \frac{e^{(1+\sigma)\sqrt{\mu}|x_i-x_j|}}{\lambda_j^{\sigma}|x_i-x_j|^{\sigma}}\varepsilon_{ij} \le \frac{e^{(1+\sigma)\sqrt{\mu}\lambda_j^{-\alpha}}}{\lambda_j^{\sigma}|x_i-x_j|^{\sigma}}\varepsilon_{ij}$$
$$\le \frac{C\mu^{\sigma T}}{\lambda_j^{\sigma}}\varepsilon_{ij} \le \frac{C}{\lambda_j^{\sigma/2}}\varepsilon_{ij} = O\Big(\frac{1}{\lambda_j^{1+\bar\sigma}} + \varepsilon_{ij}^{1+\bar\sigma}\Big).$$

□

For the expansions of the derivatives of $I\big(\sum_{j=1}^k V_{x_j,\lambda_j}\big)$, we have

Proposition B.4. *Suppose that* $N = 3$, $\lambda_i \sim e^{\frac{\bar B_1\sqrt{\mu}}{BH_m}}$ *and* $|x_i - x_j| \ge \mu^{-T}$ *for some* $T > 0$ *large. We have the following estimates:*

$$\frac{\partial}{\partial\lambda_i} I\Big(\sum_{j=1}^k U_{x_j,\lambda_j}\Big)$$
$$= -\frac{B_3\sqrt{\mu}}{\lambda_i^2} + \frac{BH(x_i)}{\lambda_i^2}\Big(\ln\frac{\lambda_i}{\sqrt{\mu}} + \gamma - \frac{1}{\lambda_j}\Big)$$
$$+ \frac{1}{\lambda_j} O\Big(\sum_{i\neq j} e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij} + \frac{1}{\lambda_j\sqrt{\mu}}\Big),$$

and

$$\frac{\partial}{\partial x_{ih}} I\Big(\sum_{j=1}^k V_{x_j,\lambda_j}\Big) = \lambda_j O\Big(\sum_{i\neq j} e^{-\sqrt{\mu}|x_i-x_j|}\varepsilon_{ij} + \frac{\ln \lambda_j}{\lambda_j}\Big).$$

Appendix C. Energy expansion, the case $N = 4$

We first recall that if $N = 4$, V_{x_j,λ_j} is the solution of

$$-\Delta v + \mu v = U^3_{x_j,\lambda_j}, \quad \text{in } \mathbb{R}^4.$$

It is easy to see that $0 < V_{x_j,\lambda_j} < U_{x_j,\lambda_j}$, V_{x_j,λ_j} is a function of $r = |y - x_j|$ and $V'_{x_j,\lambda_j} < 0$. By using the blow-up argument, we can deduce

$$V_{x_j,\lambda_j} \le \frac{C\lambda_j}{(1+\lambda_j|y-x_j|)^2}, \quad |V'_{x_j,\lambda_j}| \le \frac{C\lambda_j^2}{(1+\lambda_j|y-x_j|)^3}. \tag{C.1}$$

Let

$$\varphi_{x_j,\lambda_j} = U_{x_j,\lambda_j} - V_{x_j,\lambda_j}.$$

Then, φ_{x_j,λ_j} satisfies

$$-\Delta \varphi_{x_j,\lambda_j} + \mu \varphi_{x_j,\lambda_j} = \mu U_{x_j,\lambda_j}. \tag{C.2}$$

Denote

$$\bar\varphi(z) = \frac{\lambda_j}{\mu}\varphi_{x_j,\lambda_j}\big(\lambda_j^{-1}z + x_j\big).$$

Then,

$$-\Delta\bar\varphi + \mu\lambda_j^{-2}\bar\varphi = U, \quad \text{in } \mathbb{R}^4. \tag{C.3}$$

Writing (C.3) as

$$-(r^3\bar\varphi')' + \mu\lambda_j^{-2} r^3\bar\varphi = r^3 U,$$

we then see

$$|\bar\varphi'| \le \frac{C}{1+r}, \quad \bar\varphi \le C\ln(1+r).$$

As a result,

$$|\varphi'_{x_j,\lambda_j}| \le \frac{C\mu}{1+\lambda_j|y-x_j|}, \quad |\varphi_{x_j,\lambda_j}| \le \frac{C\mu}{\lambda_j}\ln(1+\lambda_j|y-x_j|). \tag{C.4}$$

The next lemma shows that V_{x_j,λ_j} concentrates faster than U_{x_j,λ_j}. Before we can state this lemma, we need to introduce some notation. Let $E(y)$ be the solution of

$$-\Delta E + \mu E = \delta_0, \quad \text{in } \mathbb{R}^4.$$

Then, we have

$$E(y)=\frac{1}{2\pi^2}\frac{\sqrt{\mu}}{|y|}K_1(\sqrt{\mu}|y|),$$

where $K_1(y)$ is the Bessel function. That is, $K_1(t)$ satisfies

$$t^2K''+tK'-(t^2+1)K=0,\quad t>0.$$

Note that $K_1(t)\sim t^{-\frac{1}{2}}e^{-t}$ as $t\to+\infty$, and $K_1(t)\sim t^{-1}+O(1)$ as $t\to 0$.

Denote

$$\bar K(t)=\frac{1}{2\pi^2}tK_1(t).$$

Then, $E(y)$ be be written as

$$E(y)=\frac{1}{|y|^2}\bar K(\sqrt{\mu}|y|).$$

Lemma C.1. *If $|y-x_j|\ge\lambda_j^{-1}$, then*

$$V_{x_j,\lambda_j}(y)=\frac{\bar B\bar K(\sqrt{\mu}|y-x_j|)}{\lambda_j|y-x_j|^2}+O\Big(\frac{\sqrt{\mu}}{\lambda_j^2|y-x_j|^2}+\frac{1}{\mu\lambda_j^3|y-x_j|^6}\Big),$$

where $\bar B=\int_{\mathbb{R}^4}U^3$, and $\theta>0$ is any small constant.

Proof. We have

$$V_{x_j,\lambda_j}(y)=\int_{\mathbb{R}^4}U^3_{x_j,\lambda_j}(z)E(|z-y|)\,dz.$$

Firstly,

$$\begin{aligned}&\int_{\mathbb{R}^4\setminus B_{\frac{1}{2}|y-x_j|}(x_j)}U^3_{x_j,\lambda_j}(z)E(|z-y|)\,dz\\ \le&\frac{C}{\lambda_j^3|y-x_j|^6}\int_{\mathbb{R}^4}E(|z-y|)\,dz\\ =&\frac{C'}{\lambda_j^3|y-x_j|^6}\int_0^{+\infty}t\bar K(\sqrt{\mu}t)\,dt\\ =&\frac{C'}{\mu\lambda_j^3|y-x_j|^6}\int_0^{+\infty}t\bar K(t)\,dt=O\Big(\frac{1}{\mu\lambda_j^3|y-x_j|^6}\Big).\end{aligned}$$

Secondly,

$$
\begin{aligned}
&\int_{B_{\frac{1}{2}|y-x_j|}(x_j)} U^3_{x_j,\lambda_j}(z)E(|z-y|)\,dz\\
=&\int_{B_{\frac{1}{2}|y-x_j|}(x_j)} U^3_{x_j,\lambda_j}(z)\frac{1}{|y-z|^2}\Big(\bar K(\sqrt{\mu}|y-x_j|)+O\big(\sqrt{\mu}|z-x_j|\big)\Big)\,dz\\
=&\frac{\bar K(\sqrt{\mu}|y-x_j|)}{\lambda_j|y-x_j|^2}\int_{\mathbb{R}^4}U^3+O\Big(\frac{\sqrt{\mu}}{\lambda_j^2|y-x_j|^2}\Big).
\end{aligned}
$$

So, the result follows.

□

Now we expand

$$
\begin{aligned}
I(V_{x_j,\lambda_j}) =&\frac{1}{2}\int_\Omega U^3_{x_j,\lambda_j}V_{x_j,\lambda_j}+\frac{1}{2}\int_{\partial\Omega}\frac{\partial V_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}-\frac{1}{4}\int_\Omega V^4_{x_j,\lambda_j}\\
=&\frac{1}{4}\int_\Omega U^4_{x_j,\lambda_j}+\frac{1}{2}\int_\Omega U^3_{x_j,\lambda_j}\varphi_{x_j,\lambda_j}+\frac{1}{2}\int_{\partial\Omega}\frac{\partial V_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}\\
&+O\Big(\int_\Omega U^2_{x_j,\lambda_j}\varphi^2_{x_j,\lambda_j}+\int_\Omega\varphi^4_{x_j,\lambda_j}\Big).
\end{aligned}
\tag{C.5}
$$

Lemma C.2. *There is $B_1>0$, such that*

$$
\int_{\partial\Omega}\frac{\partial V_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}=-\frac{B_1H(x_j)}{\lambda_j}+O\big(\frac{1}{\lambda_j^{1+\sigma}}\big),
$$

where $\sigma>0$ is a small constant.

Proof. It follows from (C.1) that

$$
\begin{aligned}
&\int_{\partial\Omega}\frac{\partial V_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}=\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)}\frac{\partial V_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}+\int_{\partial\Omega\setminus B_{\lambda_j^{-1/2}}(x_j)}\frac{\partial V_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}\\
=&\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)}\frac{\partial V_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}+O\Big(\int_{\partial\Omega\setminus B_{\lambda_j^{-1/2}}(x_j)}V_{x_j,\lambda_j}|V'_{x_j,\lambda_j}||y-x_j|\Big)\\
=&\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)}\frac{\partial V_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}+O\Big(\int_{\partial\Omega\setminus B_{\lambda_j^{-1/2}}(x_j)}\frac{1}{\lambda_j^2|y-x_j|^4}\Big)\\
=&\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)}\frac{\partial V_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}+O\big(\frac{1}{\lambda_j^{1+\sigma}}\big).
\end{aligned}
$$

On the other hand, by (C.1) and (C.4),

$$
\begin{aligned}
&\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} \frac{\partial V_{x_j,\lambda_j}}{\partial n}\varphi_{x_j,\lambda_j} = O\Big(\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} |V'_{x_j,\lambda_j}||y-x_j|\varphi_{x_j,\lambda_j}\Big)\\
=&O\Big(\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} \frac{\lambda_j}{\lambda_j^2|y-x_j|^2}\ln\lambda_j\Big) = O\big(\frac{1}{\lambda_j^{1+\sigma}}\big),
\end{aligned}
$$

$$
\begin{aligned}
&\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} \frac{\partial \varphi_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j} = O\Big(\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} |\varphi'_{x_j,\lambda_j}||y-x_j|V_{x_j,\lambda_j}\Big)\\
=&O\Big(\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} \frac{\mu|y-x_j|}{1+\lambda_j|y-x_j|}\frac{\lambda_j}{\lambda_j^2|y-x_j|^2}\Big) = O\big(\frac{1}{\lambda_j^{1+\sigma}}\big),
\end{aligned}
$$

and

$$
\begin{aligned}
&\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} \frac{\partial \varphi_{x_j,\lambda_j}}{\partial n}\varphi_{x_j,\lambda_j} = O\Big(\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} |\varphi'_{x_j,\lambda_j}||y-x_j|\varphi_{x_j,\lambda_j}\Big)\\
=&O\Big(\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} \ln\lambda_j\Big) = O\big(\frac{1}{\lambda_j^{1+\sigma}}\big).
\end{aligned}
$$

Moreover,

$$
\int_{\partial\Omega\cap B_{\lambda_j^{-1/2}}(x_j)} \frac{\partial U_{x_j,\lambda_j}}{\partial n}U_{x_j,\lambda_j} = -\frac{B_1H(x_j)}{\lambda_j} + O\big(\frac{1}{\lambda_j^{1+\sigma}}\big),
$$

for some small $\sigma > 0$. So the result follows. □

For the rest of this section, we always assume that $\lambda_j \sim \frac{B_3\mu\ln\mu}{BH_m}$.

Proposition C.3. *Suppose that $N = 4$. We have the following estimate:*

$$
I(V_{x_j,\lambda_j}) = A + \frac{B_3\mu\ln\lambda_j}{\lambda_j^2} - \frac{BH(x_j)}{\lambda_j} + O\Big(\frac{\mu}{\lambda_j^2}\ln\ln\mu\Big), \tag{C.6}
$$

where B_3 and B are some positive constants.

Proof. It follows from (C.5) and Lemma C.2 that

$$
\begin{aligned}
I(V_{x_j,\lambda_j}) =&\frac{1}{4}\int_\Omega U^4_{x_j,\lambda_j} + \frac{1}{2}\int_\Omega U^3_{x_j,\lambda_j}\varphi_{x_j,\lambda_j} - \frac{B_1H(x_j)}{2\lambda_j}\\
&+O\Big(\int_\Omega U^2_{x_j,\lambda_j}\varphi^2_{x_j,\lambda_j} + \int_\Omega \varphi^4_{x_j,\lambda_j} + \frac{1}{\lambda_j^{1+\sigma}}\Big).
\end{aligned} \tag{C.7}
$$

It is easy to check that there is a constant $B_2 > 0$, such that

$$\frac{1}{4}\int_\Omega U^4_{x_j,\lambda_j} = A - \frac{B_2 H(x_j)}{\lambda_j} + O\big(\frac{1}{\lambda_j^2}\big). \tag{C.8}$$

It follows from (C.4) that

$$\int_\Omega U^2_{x_j,\lambda_j}\varphi^2_{x_j,\lambda_j} = O\Big(\frac{\mu^2\ln^2\lambda_j}{\lambda_j^2}\int_\Omega U^2_{x_j,\lambda_j}\Big) = O\Big(\frac{\ln^4\mu}{\lambda_j^2}\Big), \tag{C.9}$$

and

$$\int_\Omega \varphi^4_{x_j,\lambda_j} = O\Big(\int_{B_{\lambda_j^{-1/2}(x_j)}}\varphi^4_{x_j,\lambda_j} + \int_{\Omega\setminus B_{\lambda_j^{-1/2}(x_j)}} U^4_{x_j,\lambda_j}\Big) = O\Big(\frac{\ln^4\mu}{\lambda_j^2}\Big). \tag{C.10}$$

But

$$\begin{aligned}
&\frac{1}{2}\int_\Omega U^3_{x_j,\lambda_j}\varphi_{x_j,\lambda_j} = \frac{1}{2}\int_\Omega\big(-\Delta V_{x_j,\lambda_j} + \mu V_{x_j,\lambda_j}\big)\varphi_{x_j,\lambda_j}\\
=&\frac{1}{2}\int_\Omega\big(-\Delta\varphi_{x_j,\lambda_j} + \mu\varphi_{x_j,\lambda_j}\big)V_{x_j,\lambda_j}\\
&+\frac{1}{2}\int_{\partial\Omega}\big(-\frac{\partial V_{x_j,\lambda_j}}{\partial n}\varphi_{x_j,\lambda_j} + \frac{\partial\varphi_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}\big)\\
=&\frac{1}{2}\mu\int_\Omega U_{x_j,\lambda_j}V_{x_j,\lambda_j} + \frac{1}{2}\int_{\partial\Omega}\big(-\frac{\partial V_{x_j,\lambda_j}}{\partial n}\varphi_{x_j,\lambda_j} + \frac{\partial\varphi_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}\big).
\end{aligned} \tag{C.11}$$

By (C.1), we have

$$0 \le \varphi_{x_j,\lambda_j}(y) \le U_{x_j,\lambda_j} \le \frac{C}{\lambda_j|y-x_j|^2},$$

$$\big|\varphi'_{x_j,\lambda_j}(y)\big| \le |U'_{x_j,\lambda_j}(y)| + |V'_{x_j,\lambda_j}(y)| \le \frac{C}{\lambda_j|y-x_j|^3}.$$

Using the above two relations, similar to the proof of Lemma C.2, we can obtain

$$\frac{1}{2}\int_{\partial\Omega}\big(-\frac{\partial V_{x_j,\lambda_j}}{\partial n}\varphi_{x_j,\lambda_j} + \frac{\partial\varphi_{x_j,\lambda_j}}{\partial n}V_{x_j,\lambda_j}\big) = O\big(\frac{1}{\lambda_j^{1+\sigma}}\big). \tag{C.12}$$

On the other hand,

$$
\begin{aligned}
&\int_\Omega U_{x_j,\lambda_j}V_{x_j,\lambda_j} = \int_{\Omega\cap B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}V_{x_j,\lambda_j} + \int_{\Omega\setminus B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}V_{x_j,\lambda_j}\\
=&\int_{\Omega\cap B_{\lambda_j^{-1/2}(x_j)}} U^2_{x_j,\lambda_j} + \int_{\Omega\cap B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}\varphi_{x_j,\lambda_j} + \int_{\Omega\setminus B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}V_{x_j,\lambda_j}\\
=&\frac{2B_3\ln\lambda_j}{\lambda_j^2} + O\Big(\frac{1}{\lambda_j^{2+\sigma}}\Big) + \int_{\Omega\cap B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}\varphi_{x_j,\lambda_j} + \int_{\Omega\setminus B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}V_{x_j,\lambda_j},
\end{aligned}
\tag{C.13}
$$

for some $B_3 > 0$.

It follows from (C.4) that

$$
\begin{aligned}
&\int_{\Omega\cap B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}\varphi_{x_j,\lambda_j} = O\Big(\frac{\mu\ln\lambda_j}{\lambda_j}\int_{\Omega\cap B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}\Big)\\
=&O\Big(\frac{\mu\ln\lambda_j}{\lambda_j^3}\Big).
\end{aligned}
\tag{C.14}
$$

From Lemma C.1, we find

$$
\begin{aligned}
&\int_{\Omega\setminus B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}V_{x_j,\lambda_j}\\
=&O\Big(\int_{\Omega\setminus B_{\lambda_j^{-1/2}(x_j)}} U_{x_j,\lambda_j}\Big(\frac{\bar K(\sqrt{\mu}|y-x_j|)}{\lambda_j|y-x_j|^2} + \frac{\sqrt{\mu}}{\lambda_j^2|y-x_j|^2} + \frac{1}{\mu\lambda_j^3|y-x_j|^6}\Big)\Big)\\
=&O\Big(\int_{\lambda_j^{-1/2}}^R \Big(\frac{\bar K(\sqrt{\mu}t)}{\lambda_j^2 t} + \frac{\sqrt{\mu}}{\lambda_j^3 t} + \frac{1}{\mu\lambda_j^4 t^5}\Big)\,dt\Big)\\
=&O\Big(\int_{\sqrt{\mu}\lambda_j^{-1/2}}^{\sqrt{\mu}R} \frac{\bar K(t)}{\lambda_j^2 t}\,dt + \frac{\sqrt{\mu}\ln\lambda_j}{\lambda_j^3} + \frac{1}{\mu\lambda_j^2}\Big)\\
=&O\Big(\frac{1}{\lambda_j^2}\ln\frac{\lambda_j}{\mu} + \frac{\sqrt{\mu}\ln\lambda_j}{\lambda_j^3} + \frac{1}{\mu\lambda_j^2}\Big).
\end{aligned}
\tag{C.15}
$$

So, (C.13), (C.14) and (C.15) yield

$$
\begin{aligned}
&\mu\int_\Omega U_{x_j,\lambda_j}V_{x_j,\lambda_j}\\
=&\frac{2B_3\mu\ln\lambda_j}{\lambda_j^2}+O\Big(\frac{\mu^2\ln\lambda_j}{\lambda_j^3}+\frac{\mu}{\lambda_j^2}\ln\frac{\lambda_j}{\mu}+\frac{\mu\sqrt{\mu}\ln\lambda_j}{\lambda_j^3}+\frac{1}{\lambda_j^2}\Big)\\
=&\frac{2B_3\mu\ln\lambda_j}{\lambda_j^2}+O\Big(\frac{\mu}{\lambda_j^2}\ln\ln\mu\Big),
\end{aligned}
\tag{C.16}
$$

if $\lambda_j\sim\frac{B_3\mu\ln\mu}{BH_m}$.

Combining (C.11), (C.12) and (C.16), we obtain

$$
\frac{1}{2}\int_\Omega U^3_{x_j,\lambda_j}\varphi_{x_j,\lambda_j}=\frac{B_3\mu\ln\lambda_j}{\lambda_j^2}+O\Big(\frac{\mu}{\lambda_j^2}\ln\ln\mu\Big).
\tag{C.17}
$$

So, the result follows from (C.7), (C.8), (C.9), (C.10) and (C.17). □

Proposition C.4. *We have the following estimates:*

$$
\begin{aligned}
I\big(\sum_{j=1}^k V_{x_j,\lambda_j}\big)=&\sum_{j=1}^k I\big(V_{x_j,\mu_j}\big)-B_4\sum_{i\neq j}\bar K(\sqrt{\mu}|x_i-x_j|)\varepsilon_{ij}\\
&+O\Big(\sum_{j=1}^k\frac{1}{\lambda_i^{1+\sigma}}+\sum_{i\neq j}\big(\bar K(\sqrt{\mu}|x_i-x_j|)\varepsilon_{ij}\big)^{1+\sigma}\Big)
\end{aligned}
\tag{C.18}
$$

where B_4 is a positive constant.

Proof. We have

$$
\begin{aligned}
&I\big(\sum_{j=1}^k V_{x_j,\lambda_j}\big)\\
=&\sum_{j=1}^k I\big(V_{x_j,\lambda_j}\big)+\frac{1}{2}\sum_{i<j}\int_{\partial\Omega}\frac{\partial V_{x_i,\lambda_i}}{\partial n}V_{x_j,\lambda_j}-\frac{1}{2}\sum_{i\neq j}\int_\Omega U^3_{x_i,\lambda_i}V_{x_j,\lambda_j}\\
&+O\Big(\sum_{i\neq j}\int_\Omega U^2_{x_i,\lambda_i}\varphi_{x_i,\lambda_i}U_{x_j,\lambda_j}\Big)+O\Big(\sum_{i\neq j}\varepsilon_{ij}^{1+\sigma}\Big).
\end{aligned}
\tag{C.19}
$$

Similar to (B.4), we have

$$
\begin{aligned}
&\int_\Omega U^2_{x_i,\lambda_i}\varphi_{x_i,\lambda_i}U_{x_j,\lambda_j}\\
=&O\Big(\frac{1}{\lambda_j|x_i-x_j|^2}\int_{B_{\frac12|x_i-x_j|}(x_i)}U^2_{x_i,\lambda_i}\varphi_{x_i,\lambda_i}+\frac{\varepsilon_{ij}}{\lambda_j^2|x_i-x_j|^2}\Big)\\
=&O\Big(\frac{1}{\lambda_j|x_i-x_j|^2}\frac{\mu\ln\lambda_i}{\lambda_i}\int_{B_{\frac12|x_i-x_j|\lambda_i}(0)}U^2_{x_i,\lambda_i}+\frac{\varepsilon_{ij}}{\lambda_j^2|x_i-x_j|^2}\Big)\\
=&\varepsilon_{ij}O\Big(\frac{\mu\ln^2\lambda_i}{\lambda_i^2}+\frac{1}{\lambda_j^2|x_i-x_j|^2}\Big).
\end{aligned}
\tag{C.20}
$$

On the other hand, using (C.1), we can deduce

$$
\begin{aligned}
&\int_{\partial\Omega}\frac{\partial V_{x_i,\lambda_i}}{\partial n}V_{x_j,\lambda_j}=O\big(\varepsilon_{ij}|x_i-x_j||\ln|x_i-x_j||\big)\\
=&O\big(\varepsilon_{ij}^{1+\sigma}+\frac{1}{\lambda_j^{1+\sigma}}+\frac{1}{\lambda_i^{1+\sigma}}\big).
\end{aligned}
\tag{C.21}
$$

By Lemma C.1, we find

$$
\begin{aligned}
&\int_\Omega U^3_{x_i,\lambda_i}V_{x_j,\lambda_j}\\
=&\int_{B_{\frac12|x_i-x_j|}(x_i)}U^3_{x_i,\lambda_i}\Big(\frac{\bar B\bar K(\sqrt{\mu}|y-x_j|)}{\lambda_j|y-x_j|^2}+O\Big(\frac{\sqrt{\mu}}{\lambda_j^2|y-x_j|^2}+\frac{1}{\mu\lambda_j^3|y-x_j|^6}\Big)\Big)\\
=&2B_4\bar K(\sqrt{\mu}|x_i-x_j|)\varepsilon_{ij}+O\Big(\frac{\sqrt{\mu}}{\lambda_j}+\frac{1}{\mu\lambda_j^2|x_i-x_j|^4}\Big)\varepsilon_{ij},
\end{aligned}
\tag{C.22}
$$

where B_4 is a positive constant.

Finally, we have

$$
\varepsilon_{ij}^{1+\sigma}=O\Big(\big(\bar K(\sqrt{\mu}|x_i-x_j|)\varepsilon_{ij}\big)^{1+\sigma}+\frac{1}{\lambda_j^{1+\sigma}}+\frac{1}{\lambda_i^{1+\sigma}}\Big).
\tag{C.23}
$$

In fact, if $|x_i-x_j|\ge\frac{1}{\sqrt{\mu}}$, then

$$
\varepsilon_{ij}^{1+\sigma}=\Big(\frac{1}{\lambda_i\lambda_j|x_i-x_j|^2}\Big)^{1+\sigma}=O\Big(\frac{1}{\lambda_j^{1+\sigma}}+\frac{1}{\lambda_i^{1+\sigma}}\Big).
$$

If $|x_i-x_j|\le\frac{1}{\sqrt{\mu}}$, then $\bar K(\sqrt{\mu}|x_i-x_j|)\ge c'>0$. So

$$
\varepsilon_{ij}^{1+\sigma}=O\Big(\big(\bar K(\sqrt{\mu}|x_i-x_j|)\varepsilon_{ij}\big)^{1+\sigma}\Big).
$$

Combining (C.19), (C.20), (C.21), (C.22) and (C.23), we obtain the estimate.

□

Proposition C.5. *We have the following estimates:*

$$\begin{aligned}\frac{\partial}{\partial \lambda_i} I\big(\sum_{j=1}^{k} V_{x_j,\lambda_j}\big) = &- \frac{2B_3 \mu \ln \lambda_i}{\lambda_i^3} + \frac{BH(x_i)}{\lambda_i^2} \\ &+ \lambda_i^{-1} O\Big(\sum_{i<j} \bar{K}(\sqrt{\mu}|x_i - x_j|)\varepsilon_{ij} + \sum_{j=1}^{k} \frac{\mu \ln\ln \mu}{\lambda_j^2}\Big),\end{aligned} \tag{C.24}$$

and

$$\frac{\partial}{\partial x_{ih}} I\big(\sum_{j=1}^{k} V_{x_j,\lambda_j}\big) = \lambda_i O\Big(\sum_{i<j} \bar{K}(\sqrt{\mu}|x_i - x_j|)\varepsilon_{ij} + \sum_{j=1}^{k} \frac{1}{\lambda_j}\Big), \tag{C.25}$$

Remark C.6. We can use the solution V_{x_j,λ_j} of the following linear problem

$$-\Delta v + \mu v = U_{x_j,\lambda_j}^{2^*-1}, \quad in\ \mathbb{R}^N, \quad v(+\infty) = 0$$

as the approximate solution for all the cases $N \geq 3$. It is easy to see that U_{x_j,λ_j} is the first order approximation of V_{x_j,λ_j}. For $N \geq 5$, the function U_{x_j,λ_j} concentrates fast enough so we can use it as an approximate solution instead. In the case $N = 3$, it is easy to see that

$$-\frac{c_0}{\lambda_j^{1/2}|y - x_j|}\big(1 - e^{-\sqrt{\mu}|y-x_j|}\big)$$

is the second order approximation of V_{x_j,λ_j}. So we can use $U_{x_j,\lambda_j} - \frac{c_0}{\lambda_j^{1/2}|y-x_j|}\big(1 - e^{-\sqrt{\mu}|y-x_j|}\big)$ as a better approximation for V_{x_j,λ_j} in the case $N = 3$. In the case $N = 4$, it seems it is not easy to find the second order approximation for V_{x_j,λ_j}. So, in this section, we need to calculate the energy of V_{x_j,λ_j} directly.

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