STRONGLY INTERACTING BUMPS FOR THE SCHRÖDINGER-NEWTON EQUATIONS

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Abstract. We study concentrated bound states of the Schrödinger-Newton equations

$$\begin{cases} h^2\Delta\psi - E(x)\psi + U\psi = 0, \psi > 0,\ x \in R^3, \\ \Delta U + \frac{1}{2}|\psi|^2 = 0,\ x \in R^3, \\ \psi(x) \to 0,\ U(x) \to 0 \qquad \text{as } |x| \to \infty. \end{cases}$$

Moroz, Penrose and Tod proved the existence and uniqueness of ground states of

$$\begin{cases} \Delta\psi - \psi + U\psi = 0, \psi > 0,\ x \in R^3, \\ \Delta U + \frac{1}{2}|\psi|^2 = 0,\ x \in R^3, \\ \psi(x) \to 0,\ U(x) \to 0 \qquad \text{as } |x| \to \infty. \end{cases}$$

We first prove that the linearized operator around the unique ground state radial solution (ψ_0, U_0) with

$$\psi_0(r) = \frac{Ae^{-r}}{r}(1 + o(1)) \qquad \text{as } r = |x| \to \infty,$$
$$U_0(r) = \frac{B}{r}(1 + o(1)) \quad \text{as } r = |x| \to \infty$$

for some $A, B > 0$ has a kernel whose dimension is exactly 3 (corresponding to the translational modes).

Using this result we further show: If for some positive integer K the points $P_i \in R^3$, $i = 1, 2 \ldots, K$ with $P_i \neq P_j$ for $i \neq j$ are all local minimum or local maximum or nondegenerate critical points of $E(P)$ then for h small enough there exist solutions of the Schrödinger-Newton equations with K bumps which concentrate at P_i.

We also prove that given a local maximum point P_0 of $E(P)$ there exists a solution with K bumps which all concentrate at P_0 and whose distances to P_0 are at least $O(h^{\frac{1}{3}})$.

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1. Introduction and Main Results

The Schrödinger-Newton equations were derived by Penrose [30] to describe a nonlinear system obtained by coupling the linear Schrödinger equation of quantum mechanics with the gravitation law of Newtonian mechanics. Here in the gravitation law a mass point located at the origin interacts with a matter density given by the square of the wavefunction, which is the solution of the Schrödinger equation. On the other hand, in the Schrödinger equation a given potential energy is superposed with a gravitational energy obtained by solving Newton's law of gravitation. (The Schrödinger-Newton equations have also been derived via a variational principle by Christian [5]). For a single particle of mass m, the Schrödinger-Newton equations consist of the following pair of partial differential equations

$$\begin{cases} \frac{h^2}{2m}\Delta\psi - E(x)\psi + U\psi = 0, \\ \\ \Delta U + 4\pi\gamma|\psi|^2 = 0. \end{cases} \tag{1.1}$$

Here, ψ is the wavefunction, U is the gravitational potential energy, $E(x)$ is a given external potential, $\gamma = Gm^2$, G being Newton's constant, h is Planck's constant. It is assumed that the space dimension is 3, i.e., $x \in R^3$ and Δ is the Laplace operator in R^3. We further suppose that

$$\inf_{x\in R^3} E(x) > 0,\ E(x) \in C^2(R^3). \tag{1.2}$$

The Schrödinger-Newton equations in the whole space R^3 have been studied by Moroz, Penrose and Tod [24], Moroz and Tod [25]. To state their results, we rescale U, ψ as follows

$$\psi(x) = \frac{1}{h}\left(\frac{1}{16\pi\gamma m}\right)^{1/2}\tilde{\psi}(x),\ E(x) = \frac{1}{2m}\tilde{E}(x),\ U(x) = \frac{1}{2m}\tilde{U}(x). \tag{1.3}$$

Since w.l.o.g. $\tilde{\psi}(x)$ is a real function, (1.1) reduces to the system

$$\begin{cases} h^2\Delta\tilde{\psi} - \tilde{E}(x)\tilde{\psi} + \tilde{U}\tilde{\psi} = 0, & x \in R^3, \\ \\ h^2\Delta\tilde{U} + \frac{1}{2}\tilde{\psi}^2 = 0, & x \in R^3. \end{cases} \tag{1.4}$$

Note that (1.4) is equivalent to the following non-local partial differential equation

$$h^2\Delta\tilde{\psi} - \tilde{E}(x)\tilde{\psi} + \frac{1}{8\pi h^2}\Big(\int_{R^3}\frac{\tilde{\psi}^2(\xi)}{|x-\xi|}\,d\xi\Big)\,\tilde{\psi} = 0,\ x \in R^3. \tag{1.5}$$

We are particularly interested in the semi-classical limit ($h \to 0$). The formulation (1.5) will be used for our discussion of the semi-classical limit.

From now on, we drop the tildes on $\tilde{\psi}$, $\tilde{E}(x)$, U, but we still mean the rescaled variables. The following result about (1.4) with $E(x) \equiv 1$ and $h = 1$ has been obtained by Moroz and Tod [25].

Theorem 1.1. *There exists a unique radial solution (w, u) with $w(y) \to 0$, $u(y) \to 0$ as $|y| \to \infty$, of the following problem*

$$\begin{cases} \Delta w - w + uw = 0 \ \textit{in}\ R^3, \\ \Delta u + \frac{1}{2}w^2 = 0 \ \textit{in}\ \ R^3, \\ u, w > 0,\ w(0) = \max_{y\in R^3} w(y). \end{cases} \tag{1.6}$$

Moreover, w is strictly decreasing and

$$\lim_{|y|\to\infty} w(y)e^{|y|}|y| = \lambda_0 > 0,\ \lim_{|y|\to\infty}\frac{w^{'}(y)}{w(y)} = -1 \tag{1.7}$$

for some constant $\lambda_0 > 0$ and

$$\lim_{|y|\to\infty} u(y)|y| = \lambda_1 > 0 \tag{1.8}$$

for some constant $\lambda_1 > 0$.

Remarks: 1. The solution given by Theorem 1.1 is often called the *ground state.*

2. In [25] also existence of radially symmetric solutions with $1, 2, \ldots$ zeros is proved.

3. Existence of the ground state was also proved by P. L. Lions using variational methods [20, 21].

In other words, Theorem 1.1 establishes existence of a single-peaked solution in R^3. It can be considered as the quantum-mechanic representation of a particle under the influence of gravity which is placed at the origin. A natural question to ask is the following: For a single material particle of mass m, are there any multiple-bump bound states? If yes, how do the different bumps interact?

In this paper we answer these questions. We rigorously prove that for an inhomogeneous external potential $E(x)$, multiple-bump bound states do occur. Furthermore, there is strong interaction between each pair of bumps and also between each bump and the external potential. In the semi-classical limit ($h \to 0$) these K bumps behave like K particles (mass points) located at points $P_1, \ldots, P_K$ such that their mutual attractive forces are balanced by a force which the potential $E(x)$ exerts on each individual particle. The mathematical formulation of this result is given in Theorem 1.3 below.

Our approach can be summarized as follows: We first study the kernel of the linearized operator at the ground state of (1.6) and show by an analysis which for a system of partial differential equations is by no means trivial that its dimension is exactly 3 (thus comprising exactly the three translational modes). Then we use the Liapunov-reduction scheme to reduce the problem from the system of partial differential equations on an infinite-dimensional Sobolev space to a critical point problem on the $3K$-dimensional space of the locations of the K peaks. We solve this reduced problem by a simple perturbation argument.

The following two are our main results:

Theorem 1.2. *Assume that $E(x)$ satisfies the assumption (1.2). Suppose that for a positive integer K, $P_i \in R^3$, $i = 1, \ldots, K$ are given with $P_i \neq P_j$ for $i \neq j$. Furthermore, suppose that P_i are local minimum points of $E(P)$, i.e. there exist bounded open sets Γ_i such that*

$$P_i \in \Gamma_i, E(P_i) = \min_{x \in \Gamma_i} E(x) < E(P), \forall P \in \Gamma_i \backslash \{P_i\}. \tag{1.9}$$

Then there exists $h_0 > 0$ such that for any $h < h_0$ there exists a positive solution ψ_h of (1.5) with the following properties:

(1) ψ_h has exactly K local maximum points $Q_1^h, ..., Q_K^h$ and $Q_i^h \to P_i$ as $h \to 0$.

(2) $\psi_h(x) \leq Ce^{-\beta \frac{\min_{i=1,\ldots,K} |x - Q_i^h|}{h}}$ for some $\beta > 0, C > 0$ and $\psi_h(Q_i^h) \to \alpha, \alpha > 0, i = 1, ..., K$ as $h \to 0$, i.e. ψ_h concentrates at $Q_1^h, ..., Q_K^h$.

Remark: The approach can be easily extended to the case where $P_1, ..., P_K \in R^3$ with $P_i \neq P_j$ for $i \neq j$ are all (not necessarily strict) local maxima or local minima of $E(P)$ or if they are all nondegenerate critical points of $E(P)$.

Theorem 1.3. *Assume that $E(x)$ satisfies the assumption (1.2). Let P_0 be a local maximum point of the potential $E(x)$, i.e. there exists a bounded open set Γ such that*

$$P_0 \in \Gamma, E(P_0) = \max_{x \in \Gamma} E(x) > E(P), \forall P \in \Gamma \backslash \{P_0\}. \tag{1.10}$$

Then for any positive integer $K \in \mathbb{Z}$, there exists $h_0 > 0$ such that for any $h < h_0$ there is a positive solution ψ_h of (1.5) with the following properties:

(1) ψ_h has exactly K local maximum points $Q_1^h, ..., Q_K^h$ and $Q_i^h \to P_0$ as $h \to 0$. Moreover,

$$|Q_i^h - Q_j^h| \geq Ch^{1/3}, i \neq j, i, j = 1, ..., K$$

for some $C > 0$, as $h \to 0$;

(2) $\psi_h(x) \leq Ce^{-\beta \frac{\min_{i=1,...,K} |x - Q_i^h|}{h}}$ for some $\beta > 0, C > 0$ and $\psi_h(Q_i^h) \to \alpha$, $\alpha > 0$, $i = 1, ..., K$ as $h \to 0$, i.e. ψ_h concentrates at $Q_1^h, ..., Q_K^h$.

Remarks: 1. We call the solution ψ_h given in one of the previous theorems a K-bump solution since it has the properties (1) and (2) stated there.

2. It can be shown that in the system (1.4) the corresponding solution u_h of the second equation also is a K-bump solution. However, in contrast to ψ_h, it has only algebraic decay at infinity:

$$u_h \sim \frac{C}{r}$$

for some $C > 0$ in accordance with Theorem 1.1.

3. A simple analysis of the functional

$$M_h(\mathbf{P}) = C \sum_{i=1}^{K} E(P_i)^{3/2} - Dh \sum_{i \neq j} \sum_{j=1}^{K} E(P_i)^{1/2} E(P_j)^{1/2} \frac{1}{|P_i - P_j|} + O(h^2)$$

with $C, D > 0$ given real constants (see Section 5 for its derivation and also the proof of its smoothness) noting that

$$E(P_i) = E(P_0) + O(|P_i - P_0|^2),$$

$$\nabla_{P_i} E(P_i) = \nabla_{P_0} E(P_0) + O(|P_i - P_0|) = 0 + O(|P_i - P_0|)$$

shows that for the K-bump solutions given in Theorem 1.3

$$|P_i - P_0| \geq Ch^{1/3}.$$

In the case of a nondegenerate maximum point of $E(P)$ (see the next remark for a precise definition) we even have

$$|P_i - P_0| \sim h^{1/3},$$

and from this we get

$$|P_i - P_j| \sim h^{1/3} \quad i \neq j.$$

This result stands in marked contrast with a similar result for the Schrödinger equation. Namely, it was recently proved in [16] that $|P_i - P_j| \sim h \log \frac{1}{h}$ in the case of a nondegenerate maximum point of $E(P)$. For the Schrödinger-Newton equations the bumps are strongly coupled as their distance is bigger by the algebraic factor $h^{-2/3}$ than their respective size. However, for the Schrödinger equation their distance is bigger only by a logarithmic factor $\log \frac{1}{h}$ than their respective size.

5. If P_0 is a nondegenerate critical point of $E(P)$, i.e.

$$\det(\nabla^2 E(P))|_{P=P_0} \neq 0 \tag{1.11}$$

then for $0 < h < h_0$ the peak points P_i can are uniquely determined by solving a nondegenerate system of equations.

This result can be interpreted as analytical progress towards two fundamentally important issues of quantum mechanics:

The first issue is *quantum entanglement*, the phenomenon referred to by Schrödinger as "the essence of quantum physics". Roughly speaking, it says that in a quantum mechanical system different particles or waves interact in a very intricate manner and can not be considered as being separated from one another. Although the sum of two stationary states is again a stationary state for the (linear) Schrödinger equation alone this is no longer the case for the Schrödinger equation coupled with the gravitation law and thus quantum entanglement can be accounted for. Our results show that one mass point is enough to trigger the appearance of a wavefunction with not only one but an arbitrary number K of bumps which interact strongly. If the mass point was removed the whole wavefunction would collapse. This behavior confirms the capability of the Schrödinger-Newton equations to tackle the issue of quantum entanglement.

The second issue is *state reduction.* The Liapunov-Schmidt reduction process provides a very efficient tool to locate particles in a quantum-mechanical system under the influence of gravity even when they are strongly interacting. The physical relevance of these points in R^3 obtained by Liapunov-Schmidt reduction from the wave function lies in the fact that the single particle wavefunction if it is centered at one of those points will have maximal overlap with the multi-bump solution.

There are many studies of the nonlinear Schrödinger equation on multi-bump solutions for which the bumps interacts weakly, for example [1, 4, 6, 7, 8, 10, 11, 18, 22, 28, 29, 31, 33, 34]. For multi-bump solutions with strongly interacting bumps we refer to [2, 32] and the references therein. For the time-dependent Schrödinger-Newton equations in 2D dipole-like solutions and spinning solutions were computed numerically in [15].

The paper is organized as follows. In Section 2 we provide some preliminaries which are essential for the rest of the paper. In Section 3 we show that the dimension of the kernel of the linearized operator of (1.6) is exactly three. In Section 4 we introduce the Liapunov-Schmidt reduction process and calculate the energy of the approximate solutions obtained by the Liapunov-Schmidt scheme. Finally, in Section 5 we finish the proof of the existence of solutions using a variational approach.

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2. Preliminaries

The goal in this section is to introduce and analyze an approximate solution of (1.5). Before we do this we study two related problems which will be of importance later.

Note that (1.6) may be rewritten as a single equation for w as follows:

$$\Delta_y w(y) - w(y) + \frac{1}{8\pi}\left(\int_{R^3} \frac{w^2(z)}{|y-z|}\,dz\right)w(y) = 0,\;\; y \in R^3. \tag{2.12}$$

Now (1.6) and (2.12) are equivalent: If $w \in H^2(R^3)$ is given then u is uniquely determined by the second equation of (1.6). By the Hardy-Littlewood inequality we know that

$$\|u(y)\|_{W^{2,r}(R^3)} = \left\|\frac{1}{8\pi}\int_{R^3} \frac{w^2(z)}{|y-z|}\,dz\right\|_{W^{2,r}(R^3)}$$

$$\leq \|w^2\|_{L^q(R^3)} + \|w^2\|_{L^r(R^3)}$$

for

$$\frac{1}{q} = \frac{1}{r} + \frac{2}{3}.$$

Therefore, $u \in W^{2,r}(R^3)$ for $r > 3$. Associated with (2.12) is the following energy functional

$$I(w) = \frac{1}{2}\int_{R^3}(|\nabla w(x)|^2 + w^2(x))\,dx - \frac{1}{32\pi}\int_{R^3}\int_{R^3} \frac{w^2(x)w^2(\xi)}{|x-\xi|}\,dx\,d\xi,$$

where $w \in H^2(R^3)$.

Any critical point of $I(w)$ solves the Euler-Lagrange equation (2.12) and vice versa. We calculate

$$I(w) = \frac{1}{2}\int_{R^3}(-w(y)\Delta w(y) + w^2(y))\,dy$$

$$-\frac{1}{32\pi}\int_{R^3}\int_{R^3} \frac{w^2(y)w^2(\eta)}{|y-\eta|}\,dy\,d\eta$$

$$= \frac{1}{2}\int_{R^3} w^2(y)\frac{1}{8\pi}\int_{R^3}\frac{w^2(\eta)}{|y-\eta|}\,d\eta\,dy$$

$$-\frac{1}{32\pi}\int_{R^3}\int_{R^3}\frac{w^2(y)w^2(\eta)}{|y-\eta|}\,dy\,d\eta$$

$$= \frac{1}{32\pi}\int_{R^3}\int_{R^3}\frac{w^2(y)w^2(\eta)}{|y-\eta|}\,dy\,d\eta.$$

Now we introduce a suitably rescaled ground state function in R^3. This will be essential for the rest of the paper. For fixed $a>0$ let (w_a,u_a) be the unique radially symmetric solution with $w_a(y)\to 0, u_a(y)\to 0$ as $|y|\to\infty$, of the following problem

$$\begin{cases} \Delta w_a - a w_a + u_a w_a = 0 \text{ in } R^3, \\ \Delta u_a + \frac{1}{2}w_a^2 = 0, \text{ in } \ R^3, \\ u_a, w_a > 0, w_a(0) = \max_{y\in R^3} w_a(y). \end{cases} \tag{2.13}$$

Associated with problem (2.13) is the following energy functional

$$I_a(w_a) = \frac{1}{2}\int_{R^3}(|\nabla w_a(y)|^2 + a w_a^2(y))\,dy$$

$$-\frac{1}{32\pi}\int_{R^3}\int_{R^3}\frac{w_a^2(y)w_a^2(\eta)}{|y-\eta|}\,dy\,d\eta,$$

where $w_a \in H^2(R^3)$. In the same way as for $I(w)$ we calculate

$$I_a(w_a) = \frac{1}{32\pi}\int_{R^3}\int_{R^3}\frac{w_a^2(y)w_a^2(\eta)}{|y-\eta|}\,dy\,d\eta.$$

Note that

$$w_a(y) = a w(a^{1/2}y),$$

$$u_a(y) = a u(a^{1/2}y).$$

A simple scaling argument implies

$$I_a(w_a) = a^{3/2} I(w). \tag{2.14}$$

Our goal is to construct an approximate solution of the Schrödinger-Newton equations (1.4) which has the shape of K bumps. For this purpose we fix $\mathbf{P}=(P_1,P_2,\dots P_K)\in(R^3)^K$ with $P_i\neq P_j$ for $i\neq j$. We also introduce the notations $\mathbf{P}=(P_{j,k})$, $j=1\dots,K$, $k=1,\dots,3$ and $E_j=E(P_j)$, $j=1,\dots,K$. We introduce as a first approximation to our solution

$$\psi_{h,\mathbf{P}}(x)=\sum_{i=1}^K w_{E_i}(\frac{x-P_i}{h}),$$
$$U_h(x)=\sum_{i=1}^K u_{E_i}(\frac{x-P_i}{h}).$$

Recall from the introduction that the system (1.4) is equivalent to the non-local equation (1.5). Associated with (1.5) is the following energy functional (dropping tildes)

$$J_h(\psi)=\frac{1}{2h^3}\int_{R^3}(h^2|\nabla\psi|^2+E(x)\psi^2)\,dx$$
$$-\frac{1}{32\pi h^5}\int_{R^3}\int_{R^3}\frac{\psi^2(x)\psi^2(\xi)}{|x-\xi|}\,dx\,d\xi,$$

where

$$u\in\mathcal{E}=\{w\in H^2(R^3)|\int_{R^3}E(x)w^2(x)\,dx<\infty\}.$$

We calculate

$$J_h(\psi_{h,\mathbf{P}})=\frac{1}{2h^3}\int_{R^3}(h^2|\nabla\psi_{h,\mathbf{P}}|^2+E(x)\psi^2_{h,\mathbf{P}})\,dx$$
$$-\frac{1}{32\pi h^5}\int_{R^3}\int_{R^3}\frac{\psi^2_{h,\mathbf{P}}(x)\psi^2_{h,\mathbf{P}}(\xi)}{|x-\xi|}\,dx\,d\xi$$
$$=\frac{1}{2h^3}\int_{R^3}\left[\left|\sum_{i=1}^K\nabla_{\frac{x-P_i}{h}}w_{E_i}(\frac{x-P_i}{h})\right|^2+E(x)\left(\sum_{i=1}^K w_{E_i}(\frac{x-P_i}{h})\right)^2\right]dx$$
$$-\frac{1}{32\pi h^5}\sum_{i,j}\int_{R^3}\int_{R^3}\frac{w^2_{E_i}(\frac{x-P_i}{h})w^2_{E_j}(\frac{\xi-P_j}{h})}{|x-\xi|}\,dx\,d\xi$$
$$=\frac{1}{2h^3}\int_{R^3}\Bigg[-\sum_{i=1}^K w_{E_i}(\frac{x-P_i}{h})\Delta_{\frac{x-P_i}{h}}w_{E_i}(\frac{x-P_i}{h})$$
$$-\sum_{i\neq j}\sum_{j=1}^K w_{E_i}(\frac{x-P_i}{h})\Delta_{\frac{x-P_j}{h}}w_{E_j}(\frac{x-P_j}{h})+E(x)\sum_{i=1}^K w^2_{E_i}(\frac{x-P_i}{h})\Bigg]dx$$
$$-\frac{1}{32\pi h^5}\sum_{i=1}^K\int_{R^3}\int_{R^3}\frac{w^2_{E_i}(\frac{x-P_i}{h})w^2_{E_i}(\frac{\xi-P_i}{h})}{|x-\xi|}\,dx\,d\xi$$

$$-\frac{1}{32\pi h^5}\sum_{i\neq j}\sum_{j=1}^{K}\int_{R^3}\int_{R^3}\frac{w_{E_i}^2(\frac{x-P_i}{h})w_{E_j}^2(\frac{\xi-P_j}{h})}{|x-\xi|}\,dx\,d\xi+O(e^{-C/h})$$

$$=\frac{1}{2h^3}\int_{R^3}\left[-\sum_{i=1}^{K}w_{E_i}(\frac{x-P_i}{h})(\Delta_{\frac{x-P_i}{h}}w_{E_i}(\frac{x-P_i}{h})+E(x)w_{E_i}(\frac{x-P_i}{h}))\right]dx$$

$$-\frac{1}{32\pi h^5}\sum_{i=1}^{K}\int_{R^3}\int_{R^3}\frac{w_{E_i}^2(\frac{x-P_i}{h})w_{E_i}^2(\frac{\xi-P_i}{h})}{|x-\xi|}\,dx\,d\xi$$

$$-\frac{1}{32\pi}h\sum_{i\neq j}\sum_{j=1}^{K}\frac{1}{|P_i-P_j|}E_i^{1/2}E_j^{1/2}\left(\int_{R^3}w^2(y)\,dy\right)^2$$

$$+O(e^{-C/h}+\sum_{i\neq j}\sum_{j=1}^{K}\frac{h^2}{|P_i-P_j|^2})\ \text{ as } h\to 0.$$

Here we have used that for $i\neq j$

$$\int_{R^3}w_{E_i}(\frac{x-P_i}{h})\Delta_{\frac{x-P_j}{h}}w_{E_j}(\frac{x-P_j}{h})\,dx=O(e^{-C/h})$$

(because of the exponential decay of w at infinity) and that for $i\neq j$

$$\frac{1}{32\pi h^5}\int_{R^3}\int_{R^3}\frac{w_{E_i}^2(\frac{x-P_i}{h})w_{E_j}^2(\frac{\xi-P_j}{h})}{|x-\xi|}\,dx\,d\xi$$

$$=\frac{1}{32\pi}\frac{h}{|P_i-P_j|}\left(\int_{R^3}w_{E_i}^2(y)\,dy\right)\left(\int_{R^3}w_{E_j}^2(y)\,dy\right)$$

$$+O(\frac{h^2}{|P_i-P_j|^2}).$$

We now use (2.13), (2.14) and calculate

$$J_h(\psi_{h,\mathbf{P}})=\frac{1}{2h^3}\int_{R^3}\sum_{i=1}^{K}(E(x)-E(P_i))w_{E_i}^2(\frac{x-P_i}{h})\,dx$$

$$+\frac{1}{32\pi h^5}\sum_{i=1}^{K}\int_{R^3}\int_{R^3}\frac{w_{E_i}^2(\frac{x-P_i}{h})w_{E_i}^2(\frac{\xi-P_i}{h})}{|x-\xi|}\,dx\,d\xi$$

$$-\frac{1}{32\pi}\sum_{i\neq j}\sum_{j=1}^{K}\frac{h}{|P_i-P_j|}E_i^{1/2}E_j^{1/2}\left(\int_{R^3}w^2(y)\,dy\right)^2$$

$$+O(e^{-C/h}+\sum_{i\neq j}\sum_{j=1}^{K}\frac{h^2}{|P_i-P_j|^2})\ \text{ as } h\to 0$$

$$=\sum_{i=1}^{K}E_i^{3/2}I(w)$$

$$-\frac{1}{32\pi}\sum_{i\neq j}\sum_{j=1}^{K}\frac{h}{|P_i-P_j|}E_i^{1/2}E_j^{1/2}\left(\int_{R^3}w^2(y)\,dy\right)^2$$

$$+O(h^2\Delta E(P_i)+\sum_{i\neq j}\sum_{j=1}^{K}\frac{h^2}{|P_i-P_j|^2}),$$

where $\Delta E(P_i)=\sum_{j=1}^{3}\frac{\partial^2 E(P_i)}{\partial P_{i,j}^2}$, since

$$\frac{1}{h^3}\int_{R^3}(E(x)-E(P_i))w_{E_i}^2(\frac{x-P_i}{h})\,dx$$

$$=\int_{R^3}(E(P_i+hy)-E(P_i))w_{E_i}^2(y)\,dy$$

$$=\int_{R^3}(h\nabla E(P_i)\cdot y+\frac{h^2}{2}\sum_{j,k}\frac{\partial^2 E(P_i)}{\partial P_{i,j}\partial P_{i,k}}y_jy_k)w_{E_i}^2(y)\,dy+O(h^3)$$

$$=0+\frac{h^2}{2}\Delta E(P_i)\int_{R^3}y_1^2w_{E_i}^2(y)\,dy+O(h^3)$$

$$=O(h^2\Delta E(P_i)+h^3).$$

We summarize this result in the following lemma.

Lemma 2.1.

$$J_h(\psi_{h,\mathbf{P}})=\frac{1}{32\pi}\sum_{i=1}^{K}E_i^{3/2}\int_{R^3}\int_{R^3}\frac{w^2(y)w^2(\eta)}{|y-\eta|}\,dy\,d\eta$$

$$-\frac{1}{32\pi}\sum_{i\neq j}\frac{h}{|P_i-P_j|}E_i^{1/2}E_j^{1/2}\left(\int_{R^3}w^2(y)\,dy\right)^2$$

$$+O(h^2\Delta E(P_i)+\sum_{i\neq j}\sum_{j=1}^{K}\frac{h^2}{|P_i-P_j|^2}+h^3)\qquad \textit{as } h\to 0.$$

3. The linearized operator for the single-particle solution

In this section we show that the linearization of equation (1.6) around the ground state solution (w, u) has a kernel which is exactly of dimension 3 (thus comprising exactly the translational modes). This result will be the basis to the construction of multi-bump solutions by the Liapunov-Schmidt reduction method. It is summarized by the following theorem.

Theorem 3.1. *Suppose that $(\phi, \psi) \in H^2(R^3) \times H^2(R^3)$ satisfies the following eigenvalue problem*

$$\begin{cases} \Delta\phi - \phi + u\phi + w\psi = 0, \\ \Delta\psi + w\phi = 0. \end{cases} \tag{3.15}$$

Then

$$(\phi, \psi) \in span\left\{\frac{\partial(w,u)}{\partial y_j}, \quad j = 1, 2, 3\right\}. \tag{3.16}$$

Remarks:

1. Note that (3.15) is a system of PDEs, which is in contrast to the single Schrödinger equation case. A similar eigenvalue problem has been treated in [23].

2. Theorem 3.1 states for the corresponding nonlocal eigenvalue problem (with the second equation in (3.15) solved for w and the result substituted into the first equation):

Suppose that $\phi \in H^2(R^3)$ satisfies the following eigenvalue problem

$$\Delta\phi - \phi + u\phi + w\int_{R^3} \frac{w(y)\phi(\eta)}{4\pi|y - \eta|}\, d\eta = 0. \tag{3.17}$$

Then

$$\phi \in \text{span}\left\{\frac{\partial w}{\partial y_j}, \quad j = 1, 2, 3\right\}. \tag{3.18}$$

Proof: We first recall that the eigenvalues of Δ_{S^2} are given by

$$\mu_1 = 0,\ \mu_2 = \mu_3 = \mu_4 = 2,\ \mu_4 < \mu_5,\ \mu_6,\ \mu_7, \dots . \tag{3.19}$$

Let $e_i(\theta)$ be the corresponding eigenfunctions, i.e.,

$$\Delta_{S^2} e_i + \mu_i e_i = 0, \quad i = 1, 2, \ldots .$$

For any solution (ϕ, ψ) of (3.15) set

$$\phi_i(r) = \int_{S^2} \phi(r,\theta) e_i(\theta)\, d\theta,$$

$$\psi_i(r) = \int_{S^2} \psi(r,\theta) e_i(\theta)\, d\theta.$$

Recall that

$$\Delta\phi = \Delta_r \phi + \frac{\Delta_{S^2}\phi}{r^2}.$$

We calculate

$$\Delta\phi_i = \int_{S^2} \Delta_r \phi(r,\theta) e_i(\theta)\, d\theta$$

$$= \int_{S^2} (\Delta\phi - \frac{\Delta_{S^2}\phi}{r^2}) e_i(\theta)\, d\theta$$

$$= \phi_i - u\phi_i - w\phi_i + \frac{\mu_i}{r^2}\phi_i.$$

We do the same calculation for ψ_i. This gives the system

$$\begin{cases} \Delta\phi_i - \phi_i - \frac{\mu_i}{r^2}\phi_i + u\phi_i + w\psi_i = 0, \\ \Delta\psi_i - \frac{\mu_i}{r^2}\psi_i + w\phi_i = 0. \end{cases} \tag{3.20}$$

The proof will be finished by showing the following claims.

Claim 1: If $i \geq 5$ then $\phi_i \equiv \psi_i \equiv 0$.

Suppose this is not the case. We first multiply (3.20) by w' and u', respectively, where $' = \frac{\partial}{\partial r}$, and integrate over the ball B_r centered at the origin with radius r. Note that

$$\begin{cases} \Delta w' - w' + uw' + wu' = \frac{2}{r^2} w', \\ \Delta u' + ww' = \frac{2}{r^2} u'. \end{cases} \tag{3.21}$$

Integration by parts gives

$$0=\int_{B_r}(\Delta\phi_i-\phi_i-\frac{\mu_i}{r^2}\phi_i+u\phi_i)w'\,dy+\int_{B_r}ww'\psi_i\,dy$$

$$=\int_{\partial B_r}(w'\phi_i'-\phi_i w'')\,d\theta+\int_{B_r}(\Delta w'-w'+uw')\phi_i\,dy$$

$$-\int_{B_r}\frac{\mu_i}{r^2}w'\phi_i\,dy+\int_{B_r}ww'\psi_i\,dy.$$

By (3.21) we get

$$0=\int_{\partial B_r}(w'\phi_i'-\phi_i w'')\,d\theta+\int_{B_r}\frac{2-\mu_i}{r^2}w'\phi_i\,dy$$

$$-\int_{B_r}wu'\phi_i\,dy+\int_{B_r}ww'\psi_i\,dy. \tag{3.22}$$

Similarly,

$$0=\int_{B_r}(\Delta\psi_i+w\phi_i)u'\,dy-\int_{B_r}\frac{\mu_i}{r^2}\psi_i u'\,dy$$

$$=\int_{\partial B_r}(u'\psi_i'-\psi_i u'')\,d\theta+\int_{B_r}(\Delta u'\psi_i+w\phi_i u')\,dy-\int_{B_r}\frac{\mu_i}{r^2}\psi_i u'\,dy.$$

By (3.21) we get

$$0=\int_{\partial B_r}(u'\psi_i'-\psi_i u'')\,d\theta+\int_{B_r}\frac{2-\mu_i}{r^2}u'\psi_i\,dy$$

$$-\int_{B_r}ww'\psi_i\,dy+\int_{B_r}wu'\phi_i\,dy. \tag{3.23}$$

Adding (3.22) and (3.23) we get

$$0=\int_{\partial B_r}(w'\phi_i'-\phi_i w'')\,d\theta+\int_{\partial B_r}(u'\psi_i'-\psi_i u'')\,d\theta$$

$$+\int_{B_r}\frac{2-\mu_i}{r^2}(w'\phi_i+u'\psi_i)\,dy=I_1(r)+I_2(r)+I_3(r), \tag{3.24}$$

where $I_j(r), \quad j=1,2,3$ are defined by the last equality. We now choose an appropriate r and estimate each of the terms $I_j(r)$. By definition we have

$$\phi_i'(0)=\psi_i'(0)=0.$$

Without loss of generality we assume that there is some $r_1 > 0$ such that $\phi_i(r) < 0$ for $0 < r < r_1$ and $\phi_i(r_1) = 0$. (We choose $r_1 = \infty$ if $\phi_i < 0$ in $(0, \infty)$.) Note that by standard ODE theory $\phi_i'(r_1) > 0$.

We claim that $\psi_i(0) < 0$ for r small enough. Suppose this is not the case. Since

$$\Delta \psi_i = \frac{\mu_i}{r^2}\psi_i - w\phi_i > 0$$

$\psi_i(r)$ can not have a local maximum where $\psi_i(r) > 0$ and $0 < r < r_1$. This implies

$$\psi_i(r) > \psi_i(0) \geq 0 \qquad \text{for } r \in (0, r_1).$$

By (3.20) and (1.6), we get

$$0 > \int_{B_{r_1}} (\frac{\mu_i}{r^2}\phi_i - w\psi_i)w\, dy = \int_{B_{r_1}} w(\Delta\phi_i - \phi_i + u\phi_i)\, dy$$

$$= \int_{\partial B_{r_1}} (w\phi_i' - \phi_i w')\, d\theta = 4\pi r_1^2 w(r_1)\phi_i'(r_1) > 0.$$

This gives a contradiction. Therefore $\psi_i(0) < 0$ and so $\psi_i(r) < 0$ for r small. This implies that there is some $r_2 > 0$ such that $\psi_i(r) < 0$ for $0 < r < r_2$ and $\psi_i(r_2) = 0$. (We choose $r_2 = \infty$ if $\psi_i < 0$ in $(0, \infty)$.) Note that necessarily $\psi_i'(r_2) > 0$. From now on we distinguish three different cases.

Case 1: $r_1 = r_2$.

Set $r = r_1 = r_2$. We easily calculate

$$I_1(r) < 0, \quad I_2(r) < 0, \quad I_3(r) < 0.$$

By (3.24) this gives a contradiction.

Case 2: $r_2 < r_1$.

We easily calculate $I_3(r_2) < 0$ and $I_2(r_2) < 0$. It is more difficult to evaluate $I_1(r_2)$. We define

$$\Phi(r) = r^2\phi_i'(r)w'(r) - r^2 w''(r)\phi_i(r).$$

Then for $r_2 < r < r_1$,

$$\Phi'(r) = (r^2\phi_i')'w' - (r^2 w'')'\phi_i.$$

Now we use

$$\frac{1}{r^2}(r^2\phi_i')' - \phi_i + u\phi_i + w\psi_i = \frac{\mu_i}{r^2}\phi_i,$$

$$\frac{1}{r^2}(r^2w'')' - w' + uw' + wu' = \frac{2}{r^2}w'$$

and get

$$\Phi'(r) = r^2(\phi_i - u\phi_i - w\psi_i + \frac{\mu_i}{r^2}\phi_i)w' - r^2(w' - uw' - wu' + \frac{2}{r^2}w')\phi_i$$

$$= (\mu_i - 2)\phi_i w' - r^2ww'\psi_i + r^2wu'\phi_i > 0.$$

Suppose that $\psi_i(r) > 0$ does not hold for all $r_2 < r < r_1$. Then $\psi_i(r)$ must have a zero for some $r_3 \in (r_2, r_1)$ with $\psi_i'(r_3) < 0$ such that $\psi_i(r) > 0$ for $r \in (r_2, r_3)$. Therefore, $\psi_i(r)$ must have a local maximum in (r_2, r_3). However, this is not possible since

$$\Delta\psi_i = -w\phi_i + \frac{\mu_i}{r^2}\psi_i > 0, \quad r_2 < r < r_3.$$

This is a contradiction and so $\psi_i(r) > 0$ for all $r_2 < r < r_1$.

Putting these two facts together we conclude

$$0 > r_1^2(w'(r_1)\phi_i'(r_1) - \phi_i(r_1)w''(r_1))$$

$$= \Phi(r_1) > \Phi(r_2) = \frac{1}{4\pi}I_1(r_2).$$

By (3.24) this gives a contradiction.

Case 3: $r_1 < r_2$.

We easily calculate $I_3(r_1) < 0$ and $I_1(r_1) < 0$. It is more difficult to evaluate $I_2(r_1)$. We define

$$\Psi(r) = r^2\psi_i'(r)u'(r) - r^2u''(r)\psi_i(r).$$

Then for $r_1 < r < r_2$,

$$\Psi'(r) = (r^2u')'\psi_i' - (r^2u'')'\psi_i.$$

Now we use

$$\frac{1}{r^2}(r^2\psi_i')' + w\phi_i = \frac{\mu_i}{r^2}\psi_i,$$

$$\frac{1}{r^2}(r^2u'')' + ww' = \frac{2}{r^2}u'$$

and get

$$\Psi'(r) = r^2(-w\phi_i + \frac{\mu_i}{r^2}\psi_i)u' - r^2(-ww' + \frac{2}{r^2}u')\psi_i$$

$$= (\mu_i - 2)\psi_i u' - r^2wu'\phi_i + r^2ww'\psi_i.$$

Suppose that $\phi_i(r) > 0$ does not hold for all $r_1 < r < r_2$. Then $\phi_i(r)$ must have a zero for some $r_3 \in (r_1, r_2)$ with $\phi_i'(r_3) < 0$ such that $\phi_i(r) > 0$ for $r \in (r_1, r_3)$. We compute

$$0 < \int_{B_{r_3}\setminus B_{r_1}} (-w\psi_i + \frac{\mu_i}{r^2}\phi_i)w\, dy$$

$$= \int_{B_{r_3}\setminus B_{r_1}} w(\Delta\phi_i(r) - \phi_i + u\phi_i)\, dy$$

$$= \int_{\partial B_{r_3}} (w\phi_i' - \phi_i w')\, d\theta - \int_{\partial B_{r_1}} (w\phi_i' - \phi_i w')\, d\theta$$

$$= 4\pi r_3^2 r_3 w(r_3)\phi_i'(r_3) - 4\pi r_1^2 w(r_1)\phi_i'(r_1) < 0.$$

This is a contradiction and so $\phi_i(r) > 0$ for all $r_1 < r < r_2$.

Therefore $\Psi'(r) > 0$ for $r_1 < r < r_2$ and we get

$$\Psi(r_1) < \Psi(r_2) < 0.$$

Therefore $I_2(r_1) < 0$ and (3.24) gives a contradiction.

Claim 2: If $i = 1$, then $\phi_1 \equiv \psi_1 \equiv 0$.

Suppose this is not the case. Since $\mu_1 = 0$ we have

$$\begin{cases} \Delta\phi_1 - \phi_1 + u\phi_1 + w\psi_1 = 0, \\ \Delta\psi_1 + w\phi_1 = 0. \end{cases} \tag{3.25}$$

where

$$\phi_1 = \phi_1(r),\ \psi_1 = \psi_1(r)$$

and

$$(\phi_1, \psi_1) \in H^1(R^3) \times W^{2,q}(R^3), \quad (q > 3).$$

By definition, we have

$$\phi_1'(0) = 0,\ \psi_1'(0) = 0.$$

Without loss of generality we assume that $\phi_1(0) > 0$. We define ρ such that $\phi_1(r) > 0$, $r \in (0, \rho)$ and $\phi_1(\rho) = 0$. (If $\phi_1 > 0$ for $r \in (0, \infty)$ we set $\rho = \infty$.)

We show that then necessarily $\psi_1(\rho) > 0$. Suppose not. Then multiplying the first equation in (3.25) by w and integrating over B_r we get

$$4\pi r^2(w\phi_1' - \phi_1 w') + \int_{B_r} w^2 \psi_1 \, dy = 0, \quad 0 < r < \rho.$$

This implies

$$w^2 \left(\frac{\phi_1}{w}\right)' = w\phi_1' - \phi_1 w' < 0.$$

Therefore

$$\frac{\phi_1(r)}{w(r)} < \frac{\phi_1(0)}{w(0)} = 0$$

and thus

$$\phi_1(r) < 0 \qquad \text{for } 0 < r < \rho.$$

By the second equation in (3.25)

$$\Delta\psi_1 = -w\phi_1 > 0 \qquad \text{for } r \in (0, \rho).$$

Thus ψ_1 can not have a local maximum in $(0, \rho)$. Since $\psi_1'(0) = 0$ we therefore get $\psi_1'(r) > 0$ for $r \in (0, \rho)$. This implies $\psi_1(r) > \psi_1(0) > 0$ for $0 < r < \rho$. This is a contradiction to $\psi_1(\rho) = 0$ and so $\psi_1(0) > 0$.

Since $\phi_1(0) > 0$ we know by standard ODE theory that the dimension of the solution set of (3.25) is at most one.

On the other hand,

$$(\phi_1, \psi_1) = (2w + rw', 2(u-1) + ru')$$

is a solution to (3.25). Since the dimension of the solution set is at most one we know that any solution satisfies

$$(\phi_1, \psi_1) = c(2w + rw', 2(u-1) + ru').$$

But since $\psi_1(r) \to -2$ as $r \to \infty$, we conclude $\psi_1 \notin W^{2,q}(R^3)$, $\quad (q > 3)$. Therefore (3.25) has no solution in $H^2(R^3) \times W^{2,q}(R^3)$.

Claim 3: $(i = 2, 3, 4)$. The solution for (ϕ_2, ψ_2), (ϕ_3, ψ_3), and (ϕ_4, ψ_4), respectively, is one-dimensional.

We have to show that the solution set of

$$\begin{cases} \Delta\phi_i - \phi_i + u\phi_i + w\psi_i = \frac{2}{r^2}\phi_i, \\ \Delta\psi_i + w\phi_i = \frac{2}{r^2}\psi_i, \\ \phi_i(r), \psi_i(r) \to 0 \text{ as } r \to +\infty \end{cases} \tag{3.26}$$

is one-dimensional.

Suppose that (ϕ_i, ψ_i) solve (3.26). We must have

$$\phi_i(0) = \psi_i(0) = 0.$$

Without loss of generality we assume that $\psi_i'(0) > 0$. We will show that then also $\phi_i'(0) > 0$, which, by the linearity of (3.26), implies that the solution set of (3.26) is one-dimensional.

Suppose not, i.e., let $\phi_i'(0) \leq 0$.

Let ρ be the first zero of ψ_i'. (We set $\rho = \infty$ if $\psi_i'(r) > 0$ for $r \in (0, \infty)$.) We integrate the first equation of (3.26) by w and integrate over the ball B_r to get

$$4\pi r^2(w(r)\phi_i'(r) - \phi_i(r)w'(r)) + \int_{B_r} w^2\psi_i \, dy = \int_{B_r} \frac{2}{r^2}\phi_i w \, dy, \quad 0 < r < \rho. \tag{3.27}$$

If $\phi_i'(0) < 0$ then, since $\phi_i(0) = 0$, by continuity there exists $r_1 > 0$ such that

$$\phi_i(r) < 0, \quad 0 < r < r_1, \quad \phi_i(r_1) = 0.$$

By (3.27) we get

$$\frac{w\phi_i' - \phi_i w'}{w^2} = \left(\frac{\phi_i}{w}\right)' < 0, \quad 0 < r < \min(r_1, \rho).$$

This implies

$$0 = \frac{\phi_i(r_1)}{w(r_1)} < \frac{\phi_i(r)}{w(r)} < 0, \quad 0 < r < \min(r_1, \rho)$$

and therefore $\rho < r_1$.

If $\phi_i'(0) = 0$ then by the first equation of (3.26) we get $\phi_i''(0) = 0$. We expand ϕ_i at $r = 0$ and substitute the result into the first equation of (3.26) to obtain

$$\phi_i'''(0) = -c_0 w(0)\psi_i'(0) < 0, \quad (c_0 > 0).$$

Now we continue in the same way as for $\phi_i'(0) < 0$ since there exists $r_1 > 0$ such that

$$\phi_i(r) < 0, \quad 0 < r < r_1, \quad \phi_i(r_1) = 0.$$

Moreover, in the same way as above we show $\rho < r_1$. For $0 < r < \rho$ we calculate (noting that $\phi_i < 0$ for $< \rho < r_1$)

$$\Delta\psi_i = \frac{2}{r^2}\psi_i - w\phi_i > 0.$$

Therefore ψ_i has no local maximum and $\psi_i'(r) > \psi_i'(0) > 0$ for $0 < r < \rho$. This gives $\psi_i(\rho) > \psi_i(0)$ in contradiction with $\psi_i(\rho) = 0$. Thus we have $\rho > r_1$. On the other hand, the argument based on (3.27) gives $\rho > r_1$. So we can not have $\phi'(0) \leq 0$.

□

In the following section we will use the result in Theorem 3.1 to construct multi-particle solutions by the method of Liapunov-Schmidt reduction.

4. Liapunov-Schmidt Reduction

We construct K-bump solutions $\psi_h \in H^2(R^3)$ of the non-local partial differential equation

$$h^2\Delta\psi - E(x)\psi + \frac{1}{8\pi h^2}\left(\int_{R^3}\frac{\psi^2(\xi)}{|x-\xi|}\,d\xi\right)\psi = 0,\ x\in R^3,$$

which was given in (1.5). Fix $\mathbf{P} = (P_1, P_2, ..., P_K) \in (R^3)^K$. We set

$$w_{P_i}(x) = w_{E_i}\left(\frac{x-P_i}{h}\right), \quad u_{P_i}(x) = u_{E_i}\left(\frac{x-P_i}{h}\right). \tag{4.1}$$

Since we look for K-bump solutions of (1.5), we set

$$\psi(x) = \sum_{i=1}^{K} w_{P_i}(x) + \Phi_{h,\mathbf{P}},$$

where $\|\Phi_{h,\mathbf{P}}\|_{H^2(R^3)}$ is small.

In this section, we solve problem (1.5) up to an approximate kernel and cokernel of its linearized operator, respectively. This process is commonly called Liapunov-Schmidt reduction. Since the procedure has become standard by now, we shall only give a sketch of the proof. For more details, please see and [18] and [29]. We first introduce some notations.

Using the scaling $\hat{\psi}(y) = \psi(hy)$ we introduce the operator $S_h:\ H^2(R^3)\cap\mathcal{E} \to L^2(R^3)$ (from Section 2 recall the Hardy-Littlewood and the definition $\mathcal{E} = \{w \in H^2(R^3)|\int_{R^3} E(x)w^2(x)\,dx < \infty\}$) by

$$S_h(\hat{\psi}) = \Delta\hat{\psi} - E(hy)\hat{\psi} + T[\frac{1}{2}\hat{\psi}^2]\hat{\psi},$$

where

$$T[\frac{1}{2}\hat{\psi}^2](y) = \frac{1}{8\pi}\int_{R^3}\frac{\hat{\psi}^2(\eta)}{|y-\eta|}\,d\eta.$$

Then equation (1.5) is equivalent to the equation

$$S_h(\hat{\psi}) = 0.$$

From now on we write ψ instead of $\hat{\psi}$ but we mean the rescaled function.

To solve (1.5) we first consider the linearized operator $\tilde{L}_h[\psi] : H^2(R^3) \cap \mathcal{E} \to L^2(R^3)$ by

$$\tilde{L}_h[\psi](\Phi) = \Delta\Phi - E(hy)\Phi + T[\frac{1}{2}\psi^2]\Phi + T[\Phi\psi]\psi.$$

In the following we write $\tilde{L}_h$ instead of $\tilde{L}_h[\psi]$ for $\psi = \psi_{\epsilon,\mathbf{P}}$. We remark that the operator $\tilde{L}_h$ is self-adjoint and it is then an easy consequence (integration by parts) that the cokernel of $\tilde{L}_h$ coincides with its kernel. We choose approximate cokernel and kernel as

$$\mathcal{C}_{h,\mathbf{P}} = \mathrm{span}\{h\frac{\partial w_{P_i}}{\partial P_{i,j}} | i = 1, \dots, K,\ j = 1, \dots, 3\} \subset L^2(R^3),$$

$$\mathcal{K}_{h,\mathbf{P}} = \mathrm{span}\{h\frac{\partial w_{P_i}}{\partial P_{i,j}} | i = 1, \dots, K,\ j = 1, \dots, 3\} \subset H^2(R^3) \cap \mathcal{E}.$$

Remark: Setting $x = hy$ and differentiating the equation

$$\Delta w_{P_i}(y) - E(P_i)w_{P_i}(y) + T[\frac{1}{2}w_{P_i}^2](y)w_{P_i}(y) = 0$$

with respect to $P_{i,j}$ gives

$$\Delta h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}} - E(P_i)h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}} + T[\frac{1}{2}w_{P_i}^2(y)]h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}}$$

$$+T[w_{P_i}(y)h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}}]w_{P_i}(y) - h\frac{\partial E(P_i)}{\partial P_{i,j}}w_{P_i}(y) + O(h^2) = 0,\ y \in R^3.$$

Hence it is easy to see by using Theorem 3.1 that

$$\|h\frac{\partial w_{P_i}}{\partial P_{i,j}} + \frac{\partial w_{E_i}(y)}{\partial y_j}\|_{H^2(R^3)}$$

$$= O(h|\nabla E(P_i)|\|w_{P_i}\|_{L^2(R^3)} + h^2) = O(h|\nabla E(P_i)| + h^2). \tag{4.2}$$

Let $\pi_{h,\mathbf{P}}$ denote the projection from $L^2(R^3)$ onto $\mathcal{C}^{\perp}_{h,\mathbf{P}}$ (using the L^2 scalar product). Our goal in this section is to show that the equation

$$\pi_{h,\mathbf{P}} \circ S_h(\sum_{i=1}^{K} w_{P_i} + \Phi) = 0$$

has a unique solution $\Phi = \Phi_{h,\mathbf{P}} \in \mathcal{K}^{\perp}_{h,\mathbf{P}}$ if h is small enough. Moreover $\Phi_{h,\mathbf{P}}$ is C^1 in $\mathbf{P} = (P_1, ..., P_K)$.

As a preparation the following proposition gives the invertibility of the corresponding linearized operator.

Proposition 4.1. *Let $L_{h,\mathbf{P}} := \pi_{h,\mathbf{P}} \circ \tilde{L}_h$. Then there exist positive constants $\overline{h}$ such that for all $h \in (0, \overline{h})$ and $\mathbf{P} = (P_1, ..., P_K) \in R^{3K}$ with $|P_i - P_j| > \delta$ for $i \neq j$ and some $\delta > 0$ the map*

$$L_{h,\mathbf{P}} = \pi_{h,\mathbf{P}} \circ \tilde{L}_h : \mathcal{K}^{\perp}_{h,\mathbf{P}} \to \mathcal{C}^{\perp}_{h,\mathbf{P}}$$

is both injective and surjective. Moreover

$$\|L_{h,\mathbf{P}}\Phi\|_{L^2(R^3)} \geq C\|\Phi\|_{H^2(R^3)} \tag{4.3}$$

for all $\Phi \in \mathcal{K}^{\perp}_{h,\mathbf{P}}$.

Proof: We just mention the two most important facts:

1. By the remark above

$$\int_{R^3} h^2 \frac{\partial w_{P_i}(y)}{\partial P_{i,j}} \frac{\partial w_{P_k}(y)}{\partial P_{k,l}}\, dy = E_i^{3/2} \delta_{ik} \delta jl \int_{R^3} \left(\frac{\partial w(y)}{\partial y_1}\right)^2 dy$$

$$+O(h(|\nabla E(P_i)| + |\nabla E(P_j)|) + h^2) \quad \text{as } h \to 0.$$

This means that $h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}}$, $i = 1, \ldots, K$, $j = 1, \ldots, 3$, converge to an orthogonal system in $L^2(R^3)$ as $h \to 0$.

2. We calculate

$$\tilde{L}_h[\psi_{h,\mathbf{P}}](h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}}) = -(E(hy) - E(P_i))h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}}$$

$$+(\Delta - E(P_i) + T[\frac{1}{2}w_{P_i}^2](y))(h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}} + \frac{\partial w_{E_i}(y)}{\partial y_j})$$

$$+T[w_{P_i}(h\frac{\partial w_{P_i}}{\partial P_{i,j}} + \frac{\partial w_{E_i}}{\partial y_j})](y)w_{P_i}(y)$$

$$+T[\frac{1}{2}(\sum_{k=1}^{K} w_{P_k})^2 - \frac{1}{2}w_{P_i}^2](y)h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}}$$

$$+\sum_{k\neq i} T[(w_{P_k}h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}})](y)w_{P_i}(y)$$

$$+\sum_{k\neq i} T[(w_{P_i}h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}})](y)w_{P_k}(y)$$

$$+\sum_{k,l\neq i} T[(w_{P_k}h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}})](y)w_{P_l}(y).$$

Therefore

$$\|\tilde{L}_h(h\frac{\partial w_{P_i}(y)}{\partial P_{i,j}})\|_{L^2(R^3)} = O(h|\nabla E(P_i)| + \sum_{j\neq i} \frac{h}{|P_i - P_j|} + h^2) \tag{4.4}$$

by using the remark above and the relations

$$\|T[w_{P_i}w_{P_k}]w_{P_l}\|_{L^2(R^3)} = O(e^{-C/h}), \quad i \neq k,\, l = 1, \dots, K, \tag{4.5}$$

$$\|T[w_{P_k}\frac{\partial w_{P_i}}{\partial P_{i,j}}]w_{P_l}\|_{L^2(R^3)} = O(e^{-C/h}), \quad i \neq k,\, l = 1, \dots, K, \tag{4.6}$$

$$\|T[w_{P_i}]w_{P_k}]\|_{L^2(R^3)} = O(\frac{h}{|P_i - P_k|}), \quad i \neq k. \tag{4.7}$$

With these two facts in hand the proof can easily be completed. □

We are now in a position to solve the equation

$$\pi_{h,\mathbf{P}} \circ S_h(\sum_{i=1}^{K} w_{P_i} + \Phi) = 0, \quad \Phi \in \mathcal{K}_{h,\mathbf{P}}^{\perp}. \tag{4.8}$$

For the ansatz $\psi_{h,\mathbf{P}}$ introduced in Section 2, we first compute

$$S_h(\psi_{h,\mathbf{P}}) = h^2\Delta\psi_{h,\mathbf{P}} - E(hy)\psi_{h,\mathbf{P}} + T[\frac{1}{2}\psi_{h,\mathbf{P}}^2]\psi_{h,\mathbf{P}}$$

$$= \sum_{i=1}^{K} \Delta w_{P_i}(y) - E(hy)\sum_{i=1}^{K} w_{P_i}(y)$$

$$+T[\frac{1}{2}\sum_{i,j} w_{P_i}w_{P_j})](y)\sum_{k=1}^{K} w_{P_k}(y)$$

$$= -\sum_{i=1}^{K}(E(hy)-E(P_i))w_{P_i}(y)$$

$$+T[\frac{1}{2}\sum_{i,j\neq k} w_{P_i}w_{P_j})](y)\sum_{k=1}^{K} w_{P_k}(y).$$

In the same way as in proving (4.4) we estimate

$$\|S_h(\psi_{h,\mathbf{P}})\|_{L^2(R^3)} = O(h\sum_{i=1}^{K}|\nabla E(P_i)| + \sum_{i\neq j}\sum_{j=1}^{K}\frac{h}{|P_i-P_j|} + h^2).$$

Now note that simple computations show

$$S_h(\psi_{h,\mathbf{P}}+\Phi) = S_h(\psi_{h,\mathbf{P}}) + \tilde{L}_h(\Phi) + N_{h,\mathbf{P}}(\Phi), \tag{4.9}$$

where

$$N_{h,\mathbf{P}}(\Phi) = T[\frac{1}{2}\Phi^2]\psi_{h,\mathbf{P}} + T[\psi_{h,\mathbf{P}}\Phi]\Phi + T[\frac{1}{2}\Phi^2]\Phi.$$

It is easy to see that

$$\|N_{h,\mathbf{P}}(\Phi)\|_{L^2(R^3)} = O(\|\Phi\|^2_{H^2(R^3)})$$

for $\|\Phi\|_{H^2(R^3)} \le 1$. Therefore we have established the following Lemma.

Lemma 4.2. *For h and $\|\Phi\|_{H^2(R^3)}$ sufficiently small, we have*

$$S_h(\sum_{i=1}^{K} w_{P_i} + \Phi) = M_{h,\mathbf{P}} + \tilde{L}_h(\Phi) + N_{h,\mathbf{P}}(\Phi) \tag{4.10}$$

with

$$M_{h,\mathbf{P}} := S_h(\sum_{i=1}^{K} w_{P_i}),$$

where

$$\|M_{h,\mathbf{P}}\|_{L^2(R^3)} = O(h\sum_{i=1}^{K}|\nabla E(P_i)| + \sum_{i\neq j}\sum_{j=1}^{K}\frac{h}{|P_i-P_j|} + O(h^2))$$

and

$$\|N_{h,\mathbf{P}}(\Phi)\|_{L^2(R^3)} \le C\|\Phi\|^2_{H^2(R^3)}.$$

Next we solve (4.8). Since $L_{h,\mathbf{P}} = \tilde{L}_h|_{\mathcal{K}^{\perp}_{h,\mathbf{P}}}$ is invertible (call the inverse $L^{-1}_{h,\mathbf{P}}$) we can rewrite (4.8) as

$$\Phi = -(L^{-1}_{h,\mathbf{P}} \circ \pi_{h,\mathbf{P}})M_{h,\mathbf{P}} - (L^{-1}_{h,\mathbf{P}} \circ \pi_{h,\mathbf{P}})N_{h,\mathbf{P}}(\Phi)$$

$$\equiv G_{h,\mathbf{P}}(\Phi), \tag{4.11}$$

where the operator $G_{h,\mathbf{P}}$ is defined by the last equation for $\Phi \in H^2(R^3)$. We are going to show that the operator $G_{h,\mathbf{P}}$ is a contraction on

$$B_{h,\eta} \equiv \{\Phi \in H^2(R^3) | \|(\Phi)\|_{H^2(R^3)} < \eta\}$$

if $\eta = C_0 h(\sum_{i=1}^K |\nabla E(P_i)| + \sum_{i\neq j}\sum_{j=1}^K \frac{1}{|P_i - P_j|})$ and $C_0 > 0$ is large enough. In fact, we have

$$\|G_{h,\mathbf{P}}(\Phi)\|_{H^2(R^3)} \leq C(\|\pi_{h,\mathbf{P}} \circ N_{h,\mathbf{P}}(\Phi)\|_{L^2(R^3)} + \|\pi_{h,\mathbf{P}} \circ (M_{h,\mathbf{P}})\|_{L^2(R^3)}))$$

$$\leq C(c(\eta)\eta + h\sum_{i=1}^K |\nabla E(P_i)| + \sum_{i\neq j}\sum_{j=1}^K \frac{h}{|P_i - P_j|})$$

$$< \eta$$

where $C > 0$ is independent of $\eta > 0$ and $c(\eta) \to 0$ as $\eta \to 0$. If we choose C_0 large enough, then $G_{h,\mathbf{P}}$ is a map from $B_{h,\eta}$ to $B_{h,\eta}$. Similarly we can show

$$\|G_{h,\mathbf{P}}(\Phi) - G_{h,\mathbf{P}}(\Phi')\|_{H^2(R^3)} \leq Cc(\eta)\|\Phi - \Phi'\|_{H^2(R^3)},$$

where $c(\eta) \to 0$ as $\eta \to 0$. Therefore $G_{h,\mathbf{P}}$ is a contraction on $B_{h,\eta}$. The existence of a fixed point $\Phi = \Phi_{h,\mathbf{P}}$ now follows from the Contraction Mapping Principle and hence $\Phi_{h,\mathbf{P}}$ is a solution of (4.11).

Because of

$$\|\Phi_{h,\mathbf{P}}\|_{H^2(R^3)} \leq C(\|N_{h,\mathbf{P}}(\Phi_{h,\mathbf{P}})\|_{L^2(R^3)} + \|M_{h,\mathbf{P}}\|_{L^2(R^3)})$$

$$\leq C + h\sum_{i=1}^K |\nabla E(P_i)| + \sum_{i\neq j}\sum_{j=1}^K \frac{h}{|P_i - P_j|} + c(\eta)\|\Phi_{h,\mathbf{P}}\|_{H^2(R^3)},$$

we have

$$(1 - Cc(\eta))\|(\Phi_{h,\mathbf{P}})\|_{H^2(R^3)} \leq Ch(\sum_{i=1}^K |\nabla E(P_i)| + \sum_{i\neq j}\sum_{j=1}^K \frac{1}{|P_i - P_j|}).$$

We have thus proved the following

Lemma 4.3. *There exists* $\overline{h} > 0$ *such that for any* $0 < h < \overline{h}$ *and* $\mathbf{P} \in R^{3K}$, $\mathbf{P} = (P_1, \dots, P_K)$ *with* $P_i \in R^3$, $P_i \neq P_j$ *for* $i \neq j$, *there exists a unique* $\Phi_{h,\mathbf{P}} \in \mathcal{K}_{h,\mathbf{P}}^{\perp}$ *satisfying*

$$S_h(\sum_{i=1}^{K} w_{P_i} + \Phi_{h,\mathbf{P}}) \in \mathcal{C}_{h,\mathbf{P}}^{\perp}.$$

Furthermore, we have the estimate

$$\|\Phi_{h,\mathbf{P}}\|_{H^2(R^3)} \leq Ch(\sum_{i=1}^{K} |\nabla E(P_i)| + \sum_{i \neq j} \sum_{j=1}^{K} \frac{1}{|P_i - P_j|}). \tag{4.12}$$

Finally we note that $\Phi_{h,\mathbf{P}}$ is actually smooth in $\mathbf{P}$.

Lemma 4.4. *Let* $\Phi_{h,\mathbf{P}}$ *be defined by Lemma 4.3. Then* $\Phi_{h,\mathbf{P}} \in C^1$ *in* $\mathbf{P}$.

Proof: The proof follows along the same line as the one given in [12]. Therefore we just sketch the main argument.

Notice that it can be read off directly that the functions w_{P_i}, $\partial w_{P_i}/\partial P_{i,j}$, and $\partial^2 w_{P_i}/(\partial P_{i,j}\partial P_{i,k})$ are continuous in $\mathbf{P}$. This implies that the projection $\pi_{h,\mathbf{P}}$ is C^1 in $\mathbf{P}$.

We then decompose $\frac{\partial \Phi_{h,\mathbf{P}}}{\partial P_{i,j}}$ into two parts:

$$\left(\frac{\partial \Phi_{h,\mathbf{P}}}{\partial P_{i,j}}\right) = \left(\frac{\partial \Phi_{h,\mathbf{P}}}{\partial P_{i,j}}\right)_1 + \left(\frac{\partial \Phi_{h,\mathbf{P}}}{\partial P_{i,j}},\right)_2$$

where $\left(\frac{\partial \Phi_{h,\mathbf{P}}}{\partial P_{i,j}}\right)_1 \in \mathcal{K}_{h,\mathbf{P}}$ and $\left(\frac{\partial \Phi_{h,\mathbf{P}}}{\partial P_{i,j}}\right)_2 \in \mathcal{K}_{h,\mathbf{P}}^{\perp}$.

Then it follows first by a direct calculation that $\left(\frac{\partial \Phi_{h,\mathbf{P}}}{\partial P_{i,j}}\right)_1$ is continuous in $\mathbf{P}$. Finally, by using the theorem about the smoothness of inverse operators it follows that $\left(\frac{\partial \Phi_{h,\mathbf{P}}}{\partial P_{i,j}}\right)_2$ is also continuous in $\mathbf{P}$. The proof is finished. $\square$

5. The Existence Proof

In this section, we finish the proof of Theorem 1.3.

Fix $\mathbf{P} = (P_1, \dots, P_K) \in R^{3K}$ such that $P_i \neq P_j$ for $i \neq j$. Let $\Phi_{h,\mathbf{P}}$ be the function given by Lemma 4.3. For a given (small) $c_0 > 0$ we introduce

$$\overline{\Lambda}_h := \{\mathbf{P} \in \Gamma_0^K \ : \ |P_i - P_j| \geq c_0 h, \quad i \neq j\} \tag{5.1}$$

and define a new functional

$$M_h(\mathbf{P}) = J_h(\sum_{i=1}^K w_{P_i} + \Phi_{h,\mathbf{P}}) : \overline{\Lambda}_h \to R. \tag{5.2}$$

We first prove the following asymptotic expansion of $M_h(\mathbf{P})$.

Lemma 5.1. *For $\mathbf{P} \in \bar{\Lambda}_0$, we have*

$$M_h(\mathbf{P}) = \sum_{i=1}^K E(P_i)^{3/2} I(w)$$

$$-\frac{1}{32\pi} \sum_{i\neq j} \sum_{j=1}^K E(P_i)^{1/2} E(P_j)^{1/2} \frac{h}{|P_i - P_j|} \left(\int_{R^3} w^2(y)\, dy \right)^2$$

$$+O(h^2(\sum_{i=1}^K (|\nabla E(P_i)| + \sum_{i\neq j}\sum_{j=1}^K \frac{1}{|P_i - P_j|})^2 + h^2 \sum_{i=1}^K |\Delta E(P_i)|), \tag{5.3}$$

where w is the ground state of (1.6).

Proof: For any $\mathbf{P} \in \overline{\Lambda}_h$, we have

$$M_h(\mathbf{P}) = J_h(\sum_{i=1}^K w_{P_i}) + \int_{R^3} \tilde{L}_h(\Phi_{h,\mathbf{P}})(y) \sum_{i=1}^K w_{P_i}(y)\, dy + O(\|\Phi_{h,\mathbf{P}}\|^2_{H^1(R^3)}).$$

After integration by parts and using the calculations from the proof of Proposition 4.1 we obtain

$$M_h(\mathbf{P}) = J_h(\sum_{i=1}^K w_{P_i}) + O(h^2(\sum_{i=1}^K |\nabla E(P_i)| + \sum_{i\neq j}\sum_{j=1}^K \frac{1}{P_i - P_j|})^2)$$

$$+O(\|\Phi_{h,\mathbf{P}}\|^2_{H^1(R^3)}).$$

With Lemma 2.1 and Lemma 4.3 the claim follows. □

Proof of Theorem 1.3 : By Lemma 4.3 and Lemma 4.4, there exists h_0 such that for $0 < h < h_0$ we have a C^1 map which, to any $\mathbf{P} \in \overline{\Lambda}_h$, associates $\Phi_{h,\mathbf{P}} \in \mathcal{K}_{h,\mathbf{P}}^{\perp}$ such that

$$S_h(\sum_{i=1}^{K} w_{P_i} + \Phi_{h,\mathbf{P}}) = \sum_{k=1,\ldots,K;l=1,\ldots,3} \alpha_{kl} \frac{\partial w_{P_k}}{\partial P_{k,l}} \tag{5.4}$$

for some constants $\alpha_{kl} \in R^{3K}$.

In the same way as in [16] it can be shown that for h small the optimization problem

$$\min\{M_h(\mathbf{P}) \,:\, \mathbf{P} \in \overline{\Lambda_h}\} \tag{5.5}$$

has a solution $\mathbf{P}^h \in \Lambda_h$.

That means, we have

$$\frac{\partial M_h(\mathbf{P}^h)}{\partial P_{i,j}} = 0,\ i = 1, ..., K,\ j = 1, ..., 3.$$

Let $\Phi = \Phi_{h,\mathbf{P}^h}$ and $u_h = \sum_{i=1}^{K} w_{P_i^h} + \Phi_{h,P_1^h,\ldots,P_K^h}$. Integration by parts gives

$$\int_{R^3} [\nabla u_h \nabla \frac{\partial (w_{P_i} + \Phi_{h,P_1,\ldots,P_K})}{\partial P_{i,j}} |_{P_i = P_i^h}$$

$$+ E u_h \frac{\partial (w_{P_i} + \Phi_{h,P_1,\ldots,P_K})}{\partial P_{i,j}} |_{P_i = P_i^h} - T[\frac{1}{2} u_h^2] u_h \frac{\partial (w_{P_i} + \Phi_{h,P_1,\ldots,P_K})}{\partial P_{i,j}} |_{P_i = P_i^h}] = 0$$

for $i = 1, ..., K$ and $j = 1, ..., 3$.

Therefore we obtain

$$\sum_{k=1,\ldots,K;l=1,\ldots,3} \alpha_{kl} \int_{R^3} \frac{\partial w_{P_k^h}}{\partial P_{k,l}} \frac{\partial (w_{P_i^h} + \Phi_{h,P_1^h,\ldots,P_K^h})}{\partial P_{i,j}^h} = 0, \forall i = 1, ..., K, j = 1, ..., 3. \tag{5.6}$$

Since $\Phi_{h,P_1^h,\ldots,P_K^h} \in \mathcal{K}_{h,\mathbf{P}^h}^{\perp}$, we have that

$$\int_{R^3} h \frac{\partial w_{P_k^h}(y)}{\partial P_{k,l}^h} \frac{h \partial \Phi_{h,P_1^h,\ldots,P_K^h}(y)}{\partial P_{i,j}^h} \, dy = -h^2 \int_{R^3} \frac{\partial^2 w_{P_i^h}(y)}{\partial P_{k,l}^h \partial P_{i,j}^h} \Phi_{h,P_1^h,\ldots,P_K^h}(y) \, dy$$

$$= h^2 \| \frac{\partial^2 w_{P_i^h}}{\partial P_{k,l}^h \partial P_{i,j}^h} \|_{L^2(R^3)} \| \Phi_{h,P_1^h,\ldots,P_K^h} \|_{L^2(R^3)}$$

$$= O(h\sum_{i=1}^{K}|\nabla E(P_i^h)| + \sum_{i\neq j}\sum_{j=1}^{K}\frac{h}{|P_i^h - P_j^h|}) = O(h).$$

Note that by the Proof of Proposition 4.1

$$\int_{R^3} h\frac{\partial w_{P_k^h}(y)}{\partial P_{k,l}^h} h\frac{\partial w_{P_i^h}(y)}{\partial P_{i,j}^h}\,dy = \begin{cases} E_i^{3/2}\int_{R^3}(\frac{\partial w}{\partial y_j})^2 + o(1) \text{ if } i = k, j = l \\ \\ o(1) \text{ otherwise.} \end{cases}$$

Thus equation (5.2) becomes a system of homogeneous equations for α_{kl} and the matrix of the system is nonsingular since it is diagonally dominant. So $\alpha_{kl} \equiv 0, k = 1, ..., K, l = 1, ...3$.

Hence $\psi_h = \sum_{i=1}^{K} w_{P_i^h} + \Phi_{h,P_1^h,...,P_K^h}$ is a critical point of J_h and ψ_h satisfies (1.5).

It is easy to see that by the maximum principle $\psi_h > 0$.

This proves Theorem 1.3. □

Finally we mention that the Proof of Theorem 1.2 is the same as of Theorem 1.3 except for a small change.

Proof of Theorem 1.2: Choose in the Proof of Theorem 1.3

$$\overline{\Lambda}_h := \{\mathbf{P} \in \Gamma_1 \times \Gamma_2 \times \cdots \times \Gamma_K \,:\, |P_i - P_j| \geq c_0 h, \quad i \neq j\}$$

and we optimize the following problem as in [16]

$$\max\{M_h(\mathbf{P}) \,:\, \mathbf{P} \in \overline{\Lambda_h}\}.$$

□

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