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Convergence of SCF Sequences for the Hartree-Fock Equation

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Abstract. The Hartree-Fock equation is a fundamental equation in many-electron problems. It is of practical importance in quantum chemistry to find solutions to the Hartree-Fock equation. The self-consistent field (SCF) method is a standard numerical calculation method to solve the Hartree-Fock equation. In this paper we prove that the sequence of the functions obtained in the SCF procedure is composed of a sequence of pairs of functions that converges after multiplication by appropriate unitary matrices, which strongly ensures the validity of the SCF method. A sufficient condition for the limit to be a solution to the Hartree-Fock equation after multiplication by a unitary matrix is given, and the convergence of the corresponding density operators is also proved. The method is based mainly on the proof of approach of the sequence to a critical set of a functional, compactness of the critical set, and the proof of Łojasiewicz inequality for another functional near critical points.

1. Introduction and Statement of the Result

Let us consider a molecule with n nuclei and N electrons, where $n, N \in \mathbb{N}$. A fundamental problem in quantum chemistry is the eigenvalue problem of the Hamiltonian

$$H := -\sum_{i=1}^{N} \Delta_{x_i} - \sum_{i=1}^{N}\sum_{l=1}^{n} \frac{Z_l}{|x_i - R_l|} + \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|},$$

acting on $L^2(\mathbb{R}^{3N})$, where $x_i \in \mathbb{R}^3$ is the position of the ith electron, and R_l and Z_l are the position and the atomic number of the lth nucleus respectively. By the min-max principle (see e.g. [18]) the eigenvalue problem is equivalent to the problem to find the critical values and the critical points of

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the quadratic form $\langle \Psi, H\Psi \rangle$, where $\Psi \in H^2(\mathbb{R}^{3N})$, $\|\Psi\| = 1$. The Hartree-Fock functional is obtained by restriction of the quadratic form to the set of all Slater determinants

$$\Psi := (N!)^{-1/2} \sum_{\sigma \in S_N} (\operatorname{sgn} \sigma) \varphi_1(x_{\sigma(1)}) \cdots \varphi_N(x_{\sigma(N)}),$$

where $\varphi_i \in H^2(\mathbb{R}^3)$, $1 \leq i \leq N$ and $\langle \varphi_i, \varphi_j \rangle = \delta_{ij}$. In other words, the Hartree-Fock functional is a functional defined by $\hat{\mathcal{E}}(\Phi) := \langle \Psi, H\Psi \rangle$ for $\Phi \in \mathcal{W}$, where

$$\mathcal{W} := \left\{ \Phi = {}^t(\varphi_1, \ldots, \varphi_N) \in \bigoplus_{i=1}^{N} H^2(\mathbb{R}^3) : \langle \varphi_i, \varphi_j \rangle = \delta_{ij} \right\},$$

and Ψ is the Slater determinant constructed from $\Phi = {}^t(\varphi_1, \ldots, \varphi_N)$. Here $\bigoplus_{i=1}^N H^2(\mathbb{R}^3)$ is the Hilbert space equipped with the inner product $\sum_{i=1}^N \langle \varphi_i, (1-\Delta)^2 \tilde{\varphi}_i \rangle$ for $\Phi = {}^t(\varphi_1, \ldots, \varphi_N)$ and $\tilde{\Phi} = {}^t(\tilde{\varphi}_1, \ldots, \tilde{\varphi}_N)$. The functional $\hat{\mathcal{E}}(\Phi)$ can be written explicitly as

$$\hat{\mathcal{E}}(\Phi) = \sum_{i=1}^{N} \langle \varphi_i, h\varphi_i \rangle + \frac{1}{2} \int\int \rho(x) \frac{1}{|x-y|} \rho(y) dx dy - \frac{1}{2} \int\int \frac{1}{|x-y|} |\rho(x,y)|^2 dx dy,$$

where $h := -\Delta + V$, $V(x) := -\sum_{l=1}^{n} \frac{Z_l}{|x-R_l|}$,

$$\rho(x) := \sum_{i=1}^{N} |\varphi_i(x)|^2,$$

is the density, and

$$\rho(x,y) := \sum_{i=1}^{N} \varphi_i(x) \varphi_i^*(y),$$

is the density matrix. Here and henceforth, u^* denotes the complex conjugate for a function u. In this paper we will consider for simplicity of notation the spinless functions φ_i, although the results in this paper is trivially adapted to spin-dependent functions with only notational changes.

The critical values of the Hartree-Fock functional give approximations to the eigenvalues of H, and the corresponding critical points are used for further approximations. Let us recall the definition of critical values and critical points of a functional $\hat{\mathcal{E}}(\Phi) : \mathcal{W} \to \mathbb{R}$ (see e.g. [22, Definition 43.20]). Let $\mathcal{C}_\Phi$ be the set of all curves $c : (-1,1) \to \bigoplus_{i=1}^N H^2(\mathbb{R}^3)$ such that $c(t) \in \mathcal{W}$ for any $t \in (-1,1)$, $c(0) = \Phi$ and $c'(0)$ exists. The point $\Phi \in \mathcal{W}$ is called a critical point of $\hat{\mathcal{E}}(\Phi)$, if $d\hat{\mathcal{E}}(c(t))/dt|_{t=0} = 0$ for any $c \in \mathcal{C}_\Phi$. A real number $\Lambda \in \mathbb{R}$ is called a critical value of $\hat{\mathcal{E}}(\Phi)$ if there exists a critical point Φ' of $\hat{\mathcal{E}}(\Phi)$ such that $\Lambda = \hat{\mathcal{E}}(\Phi')$. By the method of Lagrange multipliers (see e.g. [22, Proposition 43.21] and also [1, Section 2]) we can see that Φ is a critical point of $\hat{\mathcal{E}}(\Phi)$ if and only if there exists an Hermitian matrix (ϵ_{ij}) such that Φ satisfies the equation

$$\mathcal{F}(\Phi)\varphi_i = \sum_{j=1}^N \epsilon_{ij}\varphi_j,\ 1 \le i \le N.$$

Here $\mathcal{F}(\Phi)$ is an operator called Fock operator and defined by $\mathcal{F}(\Phi) := h + R^\Phi - S^\Phi$, where R^Φ is the multiplication operator by

$$R^\Phi(x) := \sum_{i=1}^N \int |x-y|^{-1}|\varphi_i(y)|^2 dy = \sum_{i=1}^N Q_{ii}^\Phi(x),$$

with

$$Q_{ij}^\Phi(x) := \int |x-y|^{-1}\varphi_j^*(y)\varphi_i(y)dy,$$

and

$$S^\Phi := \sum_{i=1}^N S_{ii}^\Phi,$$

with

$$(S_{ij}^\Phi w)(x) := \left(\int |x-y|^{-1}\varphi_j^*(y)w(y)dy\right)\varphi_i(x),$$

for $w \in L^2(\mathbb{R}^3)$. We also define an operator $\mathcal{G}(\Phi)$ by $\mathcal{G}(\Phi) := R^\Phi - S^\Phi$. Then $\mathcal{F}(\Phi)$ can be written as $\mathcal{F}(\Phi) = h + \mathcal{G}(\Phi)$. The matrix (ϵ_{ij}) is diagonalized by an $N \times N$ unitary matrix A as $A(\epsilon_{ij})A^{-1} = \mathrm{diag}\,[\epsilon_1, \dots, \epsilon_N]$, and if we define new functions $\Phi^{\mathrm{New}} := {}^t(\varphi_1^{\mathrm{New}}, \dots, \varphi_N^{\mathrm{New}})$ by $\varphi_i^{\mathrm{New}} = \sum_{j=1}^N A_{ij}\varphi_j^{\mathrm{Old}}$ from the old one $\Phi^{\mathrm{Old}} := {}^t(\varphi_1^{\mathrm{Old}}, \dots, \varphi_N^{\mathrm{Old}})$, Φ^{New} satisfies the equation

$$\mathcal{F}(\Phi)\varphi_i = \epsilon_i\varphi_i,\ 1 \le i \le N, \tag{1.1}$$

where $(\epsilon_1, \ldots, \epsilon_N) \in \mathbb{R}^N$ and $\mathrm{diag}\,[\epsilon_1, \ldots, \epsilon_N]$ is the diagonal matrix with the diagonal elements $\epsilon_1, \ldots, \epsilon_N$. The equation (1.1) is called Hartree-Fock equation. Hence a solution Φ' to the Hartree-Fock equation is a critical point of $\hat{\mathcal{E}}(\Phi)$, and $\Lambda \in \mathbb{R}$ is a critical value of $\hat{\mathcal{E}}(\Phi)$ if and only if there exists a solution Φ' to the Hartree-Fock equation such that $\Lambda = \hat{\mathcal{E}}(\Phi')$. The Hartree-Fock equation was introduced by Fock [5] and Slater [20] independently, after Hartree [9] introduced the Hartree equation that ignored the antisymmetry with respect to exchange of variables. Hereafter, let us call the tuple $\mathbf{e} := (\epsilon_1, \ldots, \epsilon_N)$ an orbital energy, if there exists a tuple of eigenfunctions $\Phi = {}^t(\varphi_1, \ldots, \varphi_N) \in \mathcal{W}$ of $\mathcal{F}(\tilde{\Phi})$ associated with $\mathbf{e}$ for some $\tilde{\Phi} \in \mathcal{W}$, i.e. we have

$$\mathcal{F}(\tilde{\Phi})\varphi_i = \epsilon_i \varphi_i, \ i = 1 \leq i \leq N.$$

(Since we will consider sequences of the tuple in this paper, it would be more convenient to call the tuple an orbital energy than each ϵ_i.) In particular, the tuple $(\epsilon_1, \ldots, \epsilon_N)$ of the numbers in the right-hand side of the Hartree-Fock equation (1.1) is an orbital energy.

The Hartree-Fock equation can not be solved exactly even for small n and N. A standard numerical calculation method to solve the equation is the self-consistent field (SCF) method. In the SCF method we set an initial function $\Phi^0 = {}^t(\varphi_1^0, \ldots, \varphi_N^0)$ and repeat the following iterative procedure until the sequence $\{\Phi^k\}$ obtained in the procedure converges. Let $\varphi_1^{k+1}, \ldots \varphi_N^{k+1}$ be an orthonormal set of eigenfunctions of $\mathcal{F}(\Phi^k)$ associated with the N smallest eigenvalues (including multiplicity) $\epsilon_1^{k+1}, \ldots, \epsilon_N^{k+1}$, i.e. they satisfy

$$\mathcal{F}(\Phi^k)\varphi_i^{k+1} = \epsilon_i^{k+1}\varphi_i^{k+1}, \ 1 \leq i \leq N.$$

(Assume here that we can choose such eigenfunctions, which is justified under the uniform well-posedness condition introduced later.) We set the next function as $\Phi^{k+1} := {}^t(\varphi_1^{k+1}, \ldots, \varphi_N^{k+1})$. Note that the choice of the eigenfunctions is not unique, because the multiplication by a complex number with the absolute value 1 makes another eigenfunction, and if an eigenvalue is degenerated, multiplication by a unitary matrix to an orthonormal basis of the corresponding eigenspace generates another orthonormal basis. However, we suppose that particular eigenfunctions have been chosen in the SCF procedure. Note that $\mathbf{e}^k := (\epsilon_1^k, \ldots, \epsilon_N^k)$ is the orbital energy associated with Φ^k. Let us call the sequence $\{\Phi^k\}$ SCF sequence.

For the analysis of the SCF sequence it is helpful to introduce operators called density operators. For $\Phi = {}^t(\varphi_1, \ldots, \varphi_N) \in \mathcal{W}$ we define the density operator $D_\Phi \in \mathcal{L}(L^2(\mathbb{R}^3))$ by

$$(D_\Phi w)(x) := \sum_{i=1}^{N} \left(\int \varphi_i^*(y) w(y) dy \right) \varphi_i(x),$$

for $w \in L^2(\mathbb{R}^3)$. We denote by $\mathcal{P}$ the set of operators

$$\mathcal{P} := \{D \in \mathcal{T}_2 : \operatorname{Ran} D \subset H^2(\mathbb{R}^3),\ D^2 = D = D^*,\ \operatorname{Tr}(D) = N\},$$

where D^* is the adjoint operator of D and $\mathcal{T}_2$ is the set of all Hilbert-Schmidt operators in $L^2(\mathbb{R}^3)$ equipped with the norm $\|D\|_2 := (\operatorname{Tr}(D^*D))^{1/2}$ (see e.g. [17]). We can easily confirm that $D_\Phi \in \mathcal{P}$ for $\Phi \in \mathcal{W}$. For $D \in \mathcal{P}$ let us define an operator $G(D)$ by

$$(G(D)w)(x) := \operatorname{Tr}(|x-y|^{-1} D) w(x) - D(|x-y|^{-1} w(y)),$$

where $|x-y|^{-1}$ is a multiplication operator with respect to y with a parameter x, and the trace is taken with respect to y. Then we can see that

$$\mathcal{G}(\Phi) = G(D_\Phi).$$

Moreover, we have

$$\hat{\mathcal{E}}(\Phi) = \hat{E}(D_\Phi),$$

with

$$\hat{E}(D) := \operatorname{Tr}(hD) + \frac{1}{2}\operatorname{Tr}(G(D)D).$$

If $\Phi = {}^t(\varphi_1, \ldots, \varphi_N) \in \mathcal{W}$ and $\tilde{\Phi} = {}^t(\tilde{\varphi}_1, \ldots, \tilde{\varphi}_N) \in \mathcal{W}$ satisfy $D_\Phi = D_{\tilde{\Phi}}$, then Φ and $\tilde{\Phi}$ are orthonormal bases of the same space $\operatorname{Ran} D_\Phi$. Hence there exists an $N \times N$ unitary matrix A such that $A\Phi = \tilde{\Phi}$. Since the Slater determinant Ψ of Φ is written as a determinant

$$\Psi = \begin{vmatrix} \varphi_1(x_1) & \cdots & \varphi_1(x_N) \\ \vdots & \ddots & \vdots \\ \varphi_N(x_1) & \cdots & \varphi_N(x_N) \end{vmatrix},$$

we have $\tilde{\Psi} = |A|\Psi$, where $\tilde{\Psi}$ is the Slater determinant of $\tilde{\Phi}$. Therefore, the possible difference between Ψ and $\tilde{\Psi}$ is only a multiplication by a complex number with the absolute value 1. Since in the approximation of eigenfunctions of H we use Ψ rather than Φ, we can conclude that the multiplication by the unitary matrix A is not important. In addition, since $\mathcal{G}(\Phi)$ is determined by D_Φ through $\mathcal{G}(\Phi) = G(D_\Phi)$, Φ^{k+1} in the SCF sequence is determined only by D_{Φ^k}. Consequently, the convergence of the density operators D_{Φ^k} is more fundamental than that of Φ^k in a certain sense.

Convergence of the SCF sequences is rarely studied from a mathematically rigorous standpoint. An important mathematically rigorous progress has been made by Cancès and Le Bris [3]. They introduced a functional $E(D, \tilde{D}) : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$ in [3] defined by

$$E(D, \tilde{D}) := \mathrm{Tr}\,(hD) + \mathrm{Tr}\,(h\tilde{D}) + \mathrm{Tr}\,(G(D)\tilde{D}),$$

which is symmetric with respect to D and $\tilde{D}$. Let us also define a functional $\mathcal{E}(\Phi, \tilde{\Phi}) : \mathcal{W} \times \mathcal{W} \to \mathbb{R}$ by

$$\begin{aligned}
\mathcal{E}(\Phi, \tilde{\Phi}) &:= \sum_{i=1}^N \langle \varphi_i, h\varphi_i\rangle + \sum_{i=1}^N \langle \tilde{\varphi}_i, h\tilde{\varphi}_i\rangle + \sum_{i=1}^N \langle \tilde{\varphi}_i, \mathcal{G}(\Phi)\tilde{\varphi}_i\rangle \\
&= \sum_{i=1}^N \langle \varphi_i, h\varphi_i\rangle + \sum_{i=1}^N \langle \tilde{\varphi}_i, \mathcal{F}(\Phi)\tilde{\varphi}_i\rangle \\
&= \sum_{i=1}^N \langle \varphi_i, \mathcal{F}(\tilde{\Phi})\varphi_i\rangle + \sum_{i=1}^N \langle \tilde{\varphi}_i, h\tilde{\varphi}_i\rangle,
\end{aligned}$$

which is symmetric with respect to $\Phi = {}^t(\varphi_1, \ldots, \varphi_N)$ and $\tilde{\Phi} = {}^t(\tilde{\varphi}_1, \ldots, \tilde{\varphi}_N)$. Then we have

$$\mathcal{E}(\Phi, \tilde{\Phi}) = E(D_\Phi, D_{\tilde{\Phi}}).$$

Note also that $\Phi^{k+1} = {}^t(\varphi_1^{k+1}, \ldots, \varphi_N^{k+1})$ is the minimizer of $\mathcal{E}(\Phi^k, \Phi)$ with respect to $\Phi \in \mathcal{W}$. The result in [3] is that there exists a convergent subsequence $\{(D_{\Phi^{k_j}}, D_{\Phi^{k_j+1}})\}$ of the sequence $\{(D_{\Phi^k}, D_{\Phi^{k+1}})\}$ of pairs of the density operators constructed from the SCF sequence. In their analysis the fact that $E(D_{\Phi^k}, D_{\Phi^{k+1}})$ is decreasing with respect to k plays an important role. Their analysis is also based on the condition called uniform well-posedness. We say that a SCF sequence $\{\Phi^k\}$ is uniformly well posed, if the following condition (UWP) is fulfilled.

(UWP) $\mathcal{F}(\Phi^k)$ has at least N isolated eigenvalues (including multiplicity) below $\inf \sigma_{ess}(\mathcal{F}(\Phi^k))$ for any k, and there exists a constant $\gamma > 0$ such that the distance between the set of the N smallest eigenvalues (including multiplicity) of $\mathcal{F}(\Phi^k)$ and the rest of the spectrum of $\mathcal{F}(\Phi^k)$ is larger than or equal to γ for any k, where $\sigma_{ess}(B)$ is the essential spectrum of B.

Note that $\sigma_{ess}(\mathcal{F}(\Phi^k)) = [0, \infty)$ (cf. the proof of Lemma 8).

Although the result in [3] was the first mathematically rigorous important step in the study of the convergence of the SCF method, existence of a convergent subsequence is essentially rather different from convergence of the sequence itself. Another important mathematically rigorous progress has been achieved by Levitt [11] under the Galerkin discretization, i.e. finite-dimensional approximation. It is proved in [11] that $\{(D_{\Phi^k}, D_{\Phi^{k+1}})\}$ itself converges under the finite-dimensional approximation. In [11], in addition to the uniform well-posedness an inequality called Łojasiewicz inequality plays a crucial role. The Łojasiewicz inequality is the result as follows. Let $m \in \mathbb{N}$ and $f(x) : \mathbb{R}^m \to \mathbb{R}$ be an analytic function. Then for each $x_0 \in \mathbb{R}^m$ there exists a neighborhood U of x_0 and two constants $\kappa > 0$ and $\theta \in (0, 1/2]$ such that when $x \in U$,

$$|f(x) - f(x_0)|^{1-\theta} \leq \kappa \|\nabla f(x)\|.$$

In this paper we consider convergence without the discretization. The followings are the main results.

THEOREM 1. *Let $\{\Phi^k\}$ be a uniformly well posed SCF sequence such that the initial function $\Phi^0 = {}^t(\varphi_1^0, \dots, \varphi_n^0)$ satisfies*

$$\|\langle x \rangle \varphi_i^0(x)\| \leq C_0, \ 1 \leq i \leq N,$$

for some $C_0 > 0$. Then there exist Ξ^∞, $\tilde{\Xi}^\infty \in \mathcal{W}$ such that

$$\lim_{k\to\infty} \|D_{\Phi^{2k}} - D_{\Xi^\infty}\|_2 = 0,$$
$$\lim_{k\to\infty} \|D_{\Phi^{2k+1}} - D_{\tilde{\Xi}^\infty}\|_2 = 0.$$

Moreover, there exists a sequence $\{A_k\}$ of $N \times N$ unitary matrices such that

$$\lim_{k\to\infty} \|A_{2k}\Phi^{2k} - \Xi^\infty\|_{\bigoplus_{i=1}^N H^2(\mathbb{R}^3)} = 0,$$
$$\lim_{k\to\infty} \|A_{2k+1}\Phi^{2k+1} - \tilde{\Xi}^\infty\|_{\bigoplus_{i=1}^N H^2(\mathbb{R}^3)} = 0.$$

Remark 2. In practical calculations for usual molecules, a function fulfilling the decay condition is always chosen as the initial function Φ^0. Thus only the uniform well-posedness is a substantial assumption.

Since the goal of the SCF method is to find a solution to the Hartree-Fock equation, and Φ^{k+1} is a tuple of eigenfunctions of $\mathcal{F}(\Phi^k)$, we are interested in whether a tuple $\hat{\Phi}^\infty = {}^t(\hat{\varphi}_1^\infty, \dots, \hat{\varphi}_N^\infty)$ of eigenfunctions of $\mathcal{F}(\Xi^\infty)$ corresponding to the N smallest eigenvalues is a solution to the Hartree-Fock equation. (Although the choice of $\hat{\Phi}^\infty$ is not unique, assume that a particular one has been chosen.) The following theorem is concerned with this problem.

Theorem 3. *Suppose the same assumption as in Theorem 1, and let Ξ^∞ and $\tilde{\Xi}^\infty$ be as in Theorem 1. Let $\gamma > 0$ be the gap in the uniform well-posedness. Then:*

(1) The distance between the set of the N smallest eigenvalues of $\mathcal{F}(\Xi^\infty)$ (resp., $\mathcal{F}(\tilde{\Xi}^\infty)$) and the rest of the spectrum of $\mathcal{F}(\Xi^\infty)$ (resp., $\mathcal{F}(\tilde{\Xi}^\infty)$) is larger than or equal to γ. Thus $\hat{\Phi}^\infty$ as above is well defined.

(2) There exists an $N \times N$ unitary matrix A_∞ such that $\tilde{\Xi}^\infty = A_\infty \hat{\Phi}^\infty$. Moreover, if we denote by $(\hat{\epsilon}_1^\infty, \dots, \hat{\epsilon}_N^\infty)$ the eigenvalues of $\mathcal{F}(\Xi^\infty)$ associated with $\hat{\Phi}^\infty = {}^t(\hat{\varphi}_1^\infty, \dots, \hat{\varphi}_N^\infty)$, we have $\hat{\epsilon}_i^\infty = \lim_{k\to\infty} \epsilon_i^{2k+1}$, $1 \le i \le N$.

(3) If there exists an $N \times N$ unitary matrix Θ such that $\Xi^\infty = \Theta\tilde{\Xi}^\infty$, then $\hat{\Phi}^\infty$ is a solution to the Hartree-Fock equation associated with the orbital energy $(\hat{\epsilon}_1^\infty, \dots, \hat{\epsilon}_N^\infty)$.

(4) If $\hat{\Phi}^\infty$ forms an orthonormal basis of the direct sum of the eigenspaces of the N smallest eigenvalues of $\mathcal{F}(\hat{\Phi}^\infty)$, then there exists an $N \times N$ unitary matrix Θ such that $\Xi^\infty = \Theta\tilde{\Xi}^\infty$.

(5) If $D_{\hat{\Phi}^\infty} = D_{\Xi^\infty}$, then there exists an $N \times N$ unitary matrix Θ such that $\Xi^\infty = \Theta\tilde{\Xi}^\infty$.

Remark 4.

(a) The condition $D_\Phi = D_{\tilde{\Phi}}$ is equivalent to that there exists a unitary matrix $\hat{A}$ such that $\Phi = \hat{A}\tilde{\Phi}$ (cf. proof of Theorem 3 (5)). In particular, if $D_{\Xi^\infty} = D_{\tilde{\Xi}^\infty}$, then by Theorem 3 (3) we can see that $\hat{\Phi}^\infty$ is a solution to the Hartree-Fock equation.

(b) There exists a case in which the SCF sequence actually fails to converge and it oscillates between two states. In [3, Example 9] such a case is given within the Restricted Hartree-Fock (RHF) method in which the functions are spin-dependent and we impose the restriction on the tuple of functions that it consists of the same spatial functions with spin up and spin down.

In the proof of Theorem 1 the uniform well-posedness is used in order to obtain a bound of the difference between D_{Φ^k} and $D_{\Phi^{k+2}}$ by the difference between $\mathcal{E}(\Phi^k, \Phi^{k+1})$ and $\mathcal{E}(\Phi^{k+1}, \Phi^{k+2})$ (cf. Lemma 6). It also yields an upper bound of the orbital energies (cf. Lemma 8) which is needed for a uniform decay estimate of φ_i^k (cf. Lemma 12). The uniform decay is in turn used to prove that the SCF sequence approaches a critical set of $\hat{\mathcal{E}}(\Phi, \tilde{\Phi})$.

In [11] due to the discretization, the known result of the Łojasiewicz inequality for finite-dimensional cases was applicable. However, in the present result detailed infinite-dimensional analysis of functionals is needed for the proof of the Łojasiewicz inequality. For example, we need to prove that the sequence $\{(\Phi^k, \Phi^{k+1})\}$ approaches to a critical set of $\mathcal{E}(\Phi, \tilde{\Phi})$, that the critical set is a compact set, and that the Fréchet second derivatives of another auxiliary functional are Fredholm operators at points corresponding to the critical points of $\mathcal{E}(\Phi, \tilde{\Phi})$. For such analysis the viewpoint of the function Φ is more suitable than that of density operators, particularly because the Fréchet second derivative of the functional of density operators is a mapping from an operator to another and difficult to analyze. Therefore, we have to relate the analysis with respect to the function Φ to that with respect to density operators. Since for any density operator there exists a corresponding class of the function Φ in which any two functions are related by a unitary matrix, we need to choose appropriate elements from the classes to obtain a relation between estimates of density operators and those of the functions. This is achieved by Lemma 7.

The Łojasiewicz inequality was proved by Łojasiewicz [15] for analytic functions in finite-dimensional cases. In [8, Proposition 1.1] the Łojasiewicz inequality was proved for a functional whose Fréchet second derivative is an isomorphism. However, the functional in the present result does not satisfy that condition. Instead its Fréchet second derivative at a critical point is decomposed into a sum of an isomorphism and a compact operator (Actually, the first differentiation is performed using a bilinear form as in [6, 1, 2] to reduce the complexity due to the complex conjugate). This form of condition was first introduced in Fučík-Nečas-Souček-Souček [6] for some functionals to prove that the corresponding critical values are isolated points in the set of all critical values. This condition for an auxiliary functional related to the Hartree-Fock functional was proved by Ashida [1] and used to show that the number of critical values less than a constant smaller than the first energy threshold is finite. It was also a main ingredient of the proof of the fact that the set of all critical points of the Hartree-Fock functional corresponding to a critical value less than the threshold is a union of a finite number of compact connected real-analytic spaces by Ashida [2]. The way to use the Łojasiewicz inequality in this paper is following that in [11] which was introduced by Salomon [19] for the study of convergence of a scheme for time-discretized quantum control.

Finally let us mention the existence of solutions to the Hartree-Fock equation and the distribution of the critical values. Existence of a solution to the Hartree-Fock equation that minimizes the Hartree-Fock functional was proved by Lieb and Simon [13] under the assumption $N < \sum_{l=1}^{n} Z_l + 1$. It was shown by Lions [14] that if $N \leq \sum_{l=1}^{n} Z_l$, there exists a sequence of solutions to the Hartree-Fock equation such that the corresponding critical values converge to 0. Lewin [12] proved that under the same assumption there exists a sequence of solutions to the Hartree-Fock equation associated with critical values converging to the first energy threshold $J(N-1)$ which is the infimum of the Hartree-Fock functional of $N-1$ electrons. For any N, Ashida [1] showed that the set of all critical values of the Hartree-Fock functional less than $J(N-1)-\epsilon$ is finite for any $\epsilon > 0$.

This paper is organized as follows. In Section 2 we prove that the SCF sequences approach subsets of all critical points of $\mathcal{E}(\Phi, \tilde{\Phi})$. The compactness of the critical sets is shown in Section 3. In Section 4 an auxiliary functional is introduced and we prove that the Fréchet second derivative of the functional is decomposed into a sum of an isomorphism and a compact operator, if the orbital energies are tuples of negative numbers. In Section 5 we show the Łojasiewicz inequality for functionals near points at which such a decomposition is given. Finally the main theorems are proved in Section 6.

2. Closeness of SCF Sequences to Critical Sets

Let $\{\Phi^k\}$ be a uniformly well posed SCF sequence. Since Φ^{k+1} minimizes the functional $\Phi \mapsto \mathcal{E}(\Phi^k, \Phi)$ and $\mathcal{E}(\Phi, \tilde{\Phi})$ is symmetric, we have

$$\mathcal{E}(\Phi^k, \Phi^{k+1}) \leq \mathcal{E}(\Phi^k, \Phi^{k-1}) = \mathcal{E}(\Phi^{k-1}, \Phi^k),$$

so that $\mathcal{E}(\Phi^k, \Phi^{k+1})$ is decreasing (cf. [3]). Here we note that $\mathcal{G}(\Phi) = R^\Phi - S^\Phi$ is a positive operator for any $\Phi = {}^t(\varphi_1, \dots, \varphi_N) \in \bigoplus_{i=1}^N H^2(\mathbb{R}^3)$, which follows from

$$\langle w, (Q_{ii}^\Phi - S_{ii}^\Phi) w \rangle = \int |x-y|^{-1} |\hat{\Psi}_i|^2 dxdy \geq 0,$$

where $\hat{\Psi}_i := 2^{-1/2}(w(x)\varphi_i(y) - \varphi_i(x)w(y))$. Hence, we have $\mathcal{E}(\Phi^k, \Phi^{k+1}) \geq 2 \inf \sigma(h)$. Therefore, the limit $\mu := \lim_{k\to\infty} \mathcal{E}(\Phi^k, \Phi^{k+1}) \geq 2 \inf \sigma(h)$ exists. Let $\Gamma_{\gamma,\mu}$ be the set of all solutions $(\Phi, \tilde{\Phi}) \in \mathcal{W} \times \mathcal{W}$ of

$$\begin{aligned} \mathcal{F}(\tilde{\Phi})\varphi_i &= \epsilon_i \varphi_i \\ \mathcal{F}(\Phi)\tilde{\varphi}_i &= \tilde{\epsilon}_i \tilde{\varphi}_i \end{aligned} \qquad 1 \leq i \leq N,$$

fulfilling $\mathcal{E}(\Phi, \tilde{\Phi}) = \mu$ and associated with orbital energies $\mathbf{e} = (\epsilon_1, \dots, \epsilon_N) \in \mathbb{R}^N$ and $\tilde{\mathbf{e}} = (\tilde{\epsilon}_1, \dots, \tilde{\epsilon}_N) \in \mathbb{R}^N$ satisfying $\epsilon_i, \tilde{\epsilon}_i \leq -\gamma$, $1 \leq i \leq N$, where γ is the gap in the uniform well-posedness, and $\Phi = {}^t(\varphi_1, \dots, \varphi_N)$ and $\tilde{\Phi} = {}^t(\tilde{\varphi}_1, \dots, \tilde{\varphi}_N)$. The set $\Gamma_{\gamma,\mu}$ is a subset of the set of all critical points of $\mathcal{E}(\Phi, \tilde{\Phi}) : \mathcal{W} \times \mathcal{W} \to \mathbb{R}$. Let us call such a set critical set. Let

$$\begin{aligned} &d((\Phi^k, \Phi^{k+1}), \Gamma_{\gamma,\mu}) \\ &\quad := \inf_{(\Phi, \tilde{\Phi}) \in \Gamma_{\gamma,\mu}} \left(\|\Phi^k - \Phi\|_{\bigoplus_{i=1}^N H^2(\mathbb{R}^3)} + \|\Phi^{k+1} - \tilde{\Phi}\|_{\bigoplus_{i=1}^N H^2(\mathbb{R}^3)} \right), \end{aligned}$$

be the distance between (Φ^k, Φ^{k+1}) and $\Gamma_{\gamma,\mu}$ in $(\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N H^2 (\mathbb{R}^3))$. In this section our goal is to prove the following lemma.

Proposition 5. *Let $\{\Phi^k\}$ be a uniformly well posed SCF sequence such that the initial function $\Phi^0 = {}^t(\varphi_1^0, \dots, \varphi_n^0)$ satisfies*

$$\|\langle x \rangle \varphi_i^0(x)\| \leq C_0, \ 1 \leq i \leq N,$$

for some $C_0 > 0$. Then we have $\lim_{k\to\infty} d((\Phi^k, \Phi^{k+1}), \Gamma_{\gamma,\mu}) = 0$, where $\mu := \lim_{k\to\infty} \mathcal{E}(\Phi^k, \Phi^{k+1})$ and γ is the gap in the uniform well-posedness.

For the proof of Proposition 5 we prepare several lemmas. First, under the uniform well-posedness we have the following estimate (cf. [3]).

LEMMA 6. *Assume that $\{\Phi^k\}$ is a uniformly well posed SCF sequence with the gap $\gamma > 0$. Then we have*

$$\mathcal{E}(\Phi^k, \Phi^{k+1}) - \mathcal{E}(\Phi^{k+1}, \Phi^{k+2}) \geq 2^{-1}\gamma \|D_{\Phi^{k+2}} - D_{\Phi^k}\|_2^2,$$

for any $k \geq 0$.

PROOF. First by the uniform well-posedness we have

$$\begin{aligned}
&\mathcal{E}(\Phi^k, \Phi^{k+1}) - \mathcal{E}(\Phi^{k+1}, \Phi^{k+2}) \\
&\quad = \sum_{i=1}^N (\langle \varphi_i^k, \mathcal{F}(\Phi^{k+1})\varphi_i^k \rangle - \langle \varphi_i^{k+2}, \mathcal{F}(\Phi^{k+1})\varphi_i^{k+2} \rangle) \\
&\quad \geq \sum_{i=1}^N \{(\epsilon_N^{k+2} + \gamma)\|(1 - E_{k+1}(\epsilon_N^{k+2} + \gamma/2))\varphi_i^k\|^2 \\
&\qquad + \langle \varphi_i^k, \mathcal{F}(\Phi^{k+1})E_{k+1}(\epsilon_N^{k+2} + \gamma/2)\varphi_i^k \rangle - \epsilon_i^{k+2}\},
\end{aligned} \tag{2.1}$$

where $E_{k+1}(\lambda)$ is the resolution of identity of $\mathcal{F}(\Phi^{k+1})$, and we used that φ_i^{k+2} is an eigenfunction of $\mathcal{F}(\Phi^{k+1})$ associated with ith eigenvalue ϵ_i^{k+2} in ascending order. Noting that the orthogonal projection of $w \in L^2(\mathbb{R}^3)$ onto the eigenspace corresponding to the jth eigenvalue of $\mathcal{F}(\Phi^{k+1})$ is given by $\langle \varphi_j^{k+2}, w \rangle \varphi_j^{k+2}$ and $\|\varphi_i^k\| = 1$, we can calculate as

$$\|(1 - E_{k+1}(\epsilon_N^{k+2} + \gamma/2))\varphi_i^k\|^2 = 1 - \sum_{j=1}^N |\langle \varphi_j^{k+2}, \varphi_i^k \rangle|^2,$$

and

$$\langle \varphi_i^k, \mathcal{F}(\Phi^{k+1})E_{k+1}(\epsilon_N^{k+2} + \gamma/2)\varphi_i^k \rangle = \sum_{j=1}^N \epsilon_j^{k+2} |\langle \varphi_j^{k+2}, \varphi_i^k \rangle|^2.$$

Thus the right-hand side of (2.1) is bounded from below by

$$\begin{aligned}
&(\epsilon_N^{k+2} + \gamma)\sum_{i=1}^N \{(1 - \sum_{j=1}^N |\langle \varphi_j^{k+2}, \varphi_i^k \rangle|^2)\} - \sum_{i=1}^N \{\epsilon_i^{k+2}(1 - \sum_{j=1}^N |\langle \varphi_i^{k+2}, \varphi_j^k \rangle|^2)\} \\
&\quad \geq \gamma(N - \sum_{i,j=1}^N |\langle \varphi_j^{k+2}, \varphi_i^k \rangle|^2),
\end{aligned}$$

where we used $\epsilon_N^{k+2} \geq \epsilon_i^{k+2}$, $1 \leq i \leq N$. Therefore, we have

$$\mathcal{E}(\Phi^k, \Phi^{k+1}) - \mathcal{E}(\Phi^{k+1}, \Phi^{k+2}) \geq \gamma(N - \sum_{i,j=1}^{N} |\langle \varphi_j^{k+2}, \varphi_i^k \rangle|^2).$$

Hence by a direct calculation we obtain

$$\begin{aligned}
&\|D_{\Phi^{k+2}} - D_{\Phi^k}\|_2^2 \\
&\quad = \mathrm{Tr}\,(D^*_{\Phi^{k+2}} D_{\Phi^{k+2}}) - \mathrm{Tr}\,(D^*_{\Phi^{k+2}} D_{\Phi^k}) - \mathrm{Tr}\,(D^*_{\Phi^k} D_{\Phi^{k+2}}) + \mathrm{Tr}\,(D^*_{\Phi^k} D_{\Phi^k}) \\
&\quad = 2N - 2\sum_{i,j=1}^{N} |\langle \varphi_j^{k+2}, \varphi_i^k \rangle|^2 \\
&\quad \leq 2\gamma^{-1}(\mathcal{E}(\Phi^k, \Phi^{k+1}) - \mathcal{E}(\Phi^{k+1}, \Phi^{k+2})),
\end{aligned}$$

which completes the proof. □

A bound for the function Φ is obtained when Lemma 6 is combined with the following lemma. Let $\bigoplus_{i=1}^N L^2(\mathbb{R}^3)$ be the Hilbert space equipped with the inner product $\sum_{i=1}^N \langle \varphi_i, \tilde{\varphi}_i \rangle$ for $\Phi = {}^t(\varphi_1, \ldots, \varphi_N)$ and $\tilde{\Phi} = {}^t(\tilde{\varphi}_1, \ldots, \tilde{\varphi}_N)$.

LEMMA 7. *For any $\Phi = {}^t(\varphi_1, \ldots, \varphi_N) \in \mathcal{W}$ and $\tilde{\Phi} = {}^t(\tilde{\varphi}_1, \ldots, \tilde{\varphi}_N) \in \mathcal{W}$ there exist $N \times N$ unitary matrices A and $\tilde{A}$ such that*

$$\|D_\Phi - D_{\tilde{\Phi}}\|_2 \geq \|A\Phi - \tilde{A}\tilde{\Phi}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)}.$$

PROOF. Let $\hat{B}$ be the matrix whose components are given by

$$\hat{B}_{ij} = \langle \varphi_i, \tilde{\varphi}_j \rangle.$$

By the singular value decomposition (see e.g. [4, Theorem 1.6.3]) there exist $N \times N$ unitary matrices A and $\tilde{A}$ such that $\bar{A}\hat{B}({}^t\tilde{A}) = \mathrm{diag}\,[\lambda_1, \cdots \lambda_N]$, where $\bar{A}$ is the complex conjugate of A and $\lambda_1, \ldots, \lambda_N$ are nonnegative real numbers that are singular values of $\hat{B}$. Besides, since it is easily seen that $\sup_{\mathbf{c} \in \mathbb{C}^N, |\mathbf{c}|=1} |\hat{B}\mathbf{c}| \leq 1$, we have $\lambda_1, \ldots, \lambda_N \leq 1$. Thus setting $\Xi =$

${}^t(\xi_1,\dots,\xi_N) := A\Phi$ and $\tilde{\Xi} = {}^t(\tilde{\xi}_1,\dots,\tilde{\xi}_N) := \tilde{A}\tilde{\Phi}$ we obtain $\langle \xi_i, \tilde{\xi}_j\rangle = \delta_{ij}\lambda_i$. Moreover, we can easily see that $D_{A\Phi} = D_\Phi$. Hence we have

$$\begin{aligned}\|D_\Phi - D_{\tilde{\Phi}}\|_2^2 = \|D_{A\Phi} - D_{\tilde{A}\tilde{\Phi}}\|_2^2 &= 2(N - \sum_{i,j=1}^N |\langle \xi_i, \tilde{\xi}_j\rangle|^2) \\ &= 2(N - \sum_{i=1}^N \lambda_i^2) \geq 2(N - \sum_{i=1}^N \lambda_i) \\ &= 2(N - \sum_{i=1}^N \langle \xi_i, \tilde{\xi}_i\rangle) = \|\Xi - \tilde{\Xi}\|^2_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)} \\ &= \|A\Phi - \tilde{A}\tilde{\Phi}\|^2_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)},\end{aligned}$$

which completes the proof. □

For the proof of the approach of the SCF sequence to $\Gamma_{\gamma,\mu}$ we need a uniform decay estimate for the functions in the sequence. The following bound on the orbital energies is necessary for the decay estimate.

Lemma 8. *Let $\{\Phi^k\}$ be a uniformly well posed SCF sequence with the gap $\gamma > 0$. Then $\epsilon_i^k \leq -\gamma$, $1 \leq i \leq N$ for any $k \geq 1$.*

Proof. Since $\epsilon_N^k = \max\{\epsilon_1^k,\dots,\epsilon_N^k\}$, we have only to prove $\epsilon_N^k \leq -\gamma$. If we prove $\sigma_{ess}(\mathcal{F}(\Phi^{k-1})) = [0,\infty)$, by the uniform well-posedness we obviously have $\epsilon_N^k \leq \inf \sigma_{ess}(\mathcal{F}(\Phi^{k-1})) - \gamma = -\gamma$, and the proof is completed. By $\sigma_{ess}(h) = [0,\infty)$ and the Weyl's essential spectrum theorem (see e.g. [17]) we only need to prove that $\mathcal{G}(\Phi^{k-1})$ is h-compact. Since $R^{\Phi^{k-1}}(x)$ is a bounded function decaying as $|x| \to \infty$, $R^{\Phi^{k-1}}$ is Δ-compact, and thus h-compact. Because $S^{\Phi^{k-1}}$ is an integral operator of the Hilbert-Schmidt type, it is a compact operator. Consequently, $\mathcal{G}(\Phi^{k-1})$ is h-compact, which completes the proof. □

Let us define $\langle x\rangle := \sqrt{1+|x|^2}$. We denote the $L^2(\mathbb{R}^3)$ norm of $w \in L^2(\mathbb{R}^3)$ by $\|w\|$. Recall that since φ_i^{k+1} is an eigenfunction of $\mathcal{F}(\Phi^k)$ associated with the eigenvalue ϵ_i^{k+1}, we have

$$\mathcal{F}(\Phi^k)\varphi_i^{k+1} = \epsilon_i^{k+1}\varphi_i^{k+1}. \tag{2.2}$$

The following lemma gives a uniform H^1 bound for the sequence.

LEMMA 9. *For any $\nu > 0$ there exists a constant $\tilde{C}_\nu$ such that any solution $\Phi = {}^t(\varphi_1, \dots, \varphi_N) \in \mathcal{W}$ of*

$$\mathcal{F}(\tilde{\Phi})\varphi_i = \epsilon_i \varphi_i, \; 1 \le i \le N, \tag{2.3}$$

for some $\tilde{\Phi} \in \bigoplus_{i=1}^N H^2(\mathbb{R}^3)$ and $(\epsilon_1, \dots, \epsilon_N) \in \mathbb{R}^N$ with $|\epsilon_i| \le \nu, \; 1 \le i \le N$ satisfies $\|\nabla \varphi_i\| < \tilde{C}_\nu, \; 1 \le i \le N$.

REMARK 10. Assume that $\tilde{\Phi} \in \mathcal{W}$ and that Φ is a solution of (2.3) with the orbital energy $\mathbf{e} = (\epsilon_1, \dots, \epsilon_N)$ satisfying $\epsilon_i \le 0, \; 1 \le i \le N$. Then by $\mathcal{G}(\tilde{\Phi}) \ge 0$ we have

$$\epsilon_i = \langle \varphi_i, \mathcal{F}(\tilde{\Phi})\varphi_i \rangle \ge \langle \varphi_i, h\varphi_i \rangle \ge \inf \sigma(h),$$

so that Lemma 9 yields $\|\nabla \varphi_i\| < \tilde{C}_b$, where $b := |\inf \sigma(h)|$.

PROOF. By the Hardy inequality we can estimate the Coulomb potential as

$$\int \frac{1}{|x|}|w(x)|^2 dx \le \left\| \frac{1}{|x|} w(x) \right\| \|w\| \le 2\|\nabla w\| \|w\| \le \delta \|\nabla w\|^2 + \delta^{-1}\|w\|,$$

for any $w \in H^1(\mathbb{R}^3)$ and $\delta > 0$. Since the center of the Coulomb potential is irrelevant to the Hardy inequality, the potential V in h is estimated as

$$|\langle w, Vw \rangle| \le \sum_l Z_l(\delta \|\nabla w\|^2 + \delta^{-1}\|w\|^2).$$

Thus we obtain

$$\begin{aligned} \|\nabla w\|^2 &= \langle w, (-\Delta + V)w \rangle - \langle w, Vw \rangle \\ &\le \langle w, hw \rangle + \sum_l Z_l(\delta \|\nabla w\|^2 + \delta^{-1}\|w\|^2). \end{aligned}$$

If we choose δ small enough so that $\delta \sum_l Z_l < 1$ will hold, we have

$$\|\nabla w\|^2 \le C\langle w, hw \rangle + C\delta^{-1} \sum_l Z_l \|w\|^2,$$

where $C := (1 - \delta \sum_l Z_l)^{-1}$. Since $\mathcal{F}(\tilde{\Phi}) = h + \mathcal{G}(\tilde{\Phi})$ and $\mathcal{G}(\tilde{\Phi}) \geq 0$, we can see that

$$\|\nabla w\|^2 \leq C\langle w, \mathcal{F}(\tilde{\Phi})w\rangle + C\delta^{-1} \sum_l Z_l \|w\|^2. \tag{2.4}$$

Substituting $w = \varphi_i$ into (2.4) and using $\mathcal{F}(\tilde{\Phi})\varphi_i = \epsilon_i \varphi_i$, $\|\varphi_i\| = 1$ and the assumption $|\epsilon_i| < \nu$, we obtain

$$\|\nabla \varphi_i\|^2 \leq \tilde{C}_\nu^2, \ 1 \leq i \leq N,$$

where $\tilde{C}_\nu := (C\nu + C\delta^{-1} \sum_l Z_l)^{1/2}$. This completes the proof. □

The bound in Lemma 9 is fequently used in combination with the following lemma.

Lemma 11. *Let $a > 0$ be a constant. Assume that $\Phi = {}^t(\varphi_1, \ldots, \varphi_N)$, $\tilde{\Phi}^t(\tilde{\varphi}_1, \ldots, \tilde{\varphi}_N) \in \bigoplus_{i=1}^N L^2(\mathbb{R}^3)$ and $\psi, \tilde{\psi} \in L^2(\mathbb{R}^3)$ satisfy $\|\varphi_i\|_{H^1(\mathbb{R}^3)}$, $\|\tilde{\varphi}_i\|_{H^1(\mathbb{R}^3)}, \|\psi\|_{H^1(\mathbb{R}^3)}, \|\tilde{\psi}\|_{H^1(\mathbb{R}^3)} \leq a$. Then there exists a constant $C_a > 0$ such that*

$$\|\mathcal{G}(\Phi)\psi - \mathcal{G}(\tilde{\Phi})\tilde{\psi}\| \leq C_a \left(\|\Phi - \tilde{\Phi}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)} + \|\psi - \tilde{\psi}\| \right).$$

Proof. We shall estimate $S_{ii}^{\Phi}\psi - S_{ii}^{\tilde{\Phi}}\tilde{\psi}$. We have

$$\begin{aligned} S_{ii}^{\Phi}\psi - S_{ii}^{\tilde{\Phi}}\tilde{\psi} = &\left(\int |x-y|^{-1}(\varphi_i(y) - \tilde{\varphi}_i(y))\psi(y)dy \right) \varphi_i(x) \\ &+ \left(\int |x-y|^{-1}\tilde{\varphi}_i(y)(\psi(y) - \tilde{\psi}(y))dy \right) \varphi_i(x) \\ &+ \left(\int |x-y|^{-1}\tilde{\varphi}_i(y)\tilde{\psi}(y)dy \right) (\varphi_i(x) - \tilde{\varphi}_i(x)) \end{aligned}$$

Thus the Cauchy-Schwartz inequality and the Hardy inequality give

$$\|S_{ii}^{\Phi}\psi - S_{ii}^{\tilde{\Phi}}\tilde{\psi}\| \leq 4a^2\|\varphi_i - \tilde{\varphi}_i\| + 2a^2\|\psi - \tilde{\psi}\|.$$

We have a similar estimate also for $Q_{ii}^{\Phi}(x)\psi(x) - Q_{ii}^{\tilde{\Phi}}(x)\tilde{\psi}(x)$. Since $\mathcal{G}(\Phi) = \sum_i (Q_{ii}^{\Phi} - S_{ii}^{\Phi})$, we obtain the result. □

In the proof of Proposition 5 we need the following uniform decay estimate.

Lemma 12. *Let $\{\Phi^k\}$ be a uniformly well posed SCF sequence. Assume that there exists a constant $C_0 > 0$ such that*

$$\|\langle x\rangle \varphi_i^0(x)\| \le C_0,\ 1 \le i \le N.$$

Then there exists a constant $\mathcal{C} > 0$ such that

$$\|\langle x\rangle \varphi_i^k(x)\| \le \mathcal{C},\ 1 \le i \le N, \tag{2.5}$$

for any $k \ge 0$.

Proof. Let k be fixed and let us assume that there exists C_k such that

$$\|\langle x\rangle \varphi_i^k(x)\|^2 \le C_k,\ 1 \le i \le N. \tag{2.6}$$

We shall seek C_{k+1} so that (2.6) will hold with k replaced by $k+1$. Let $\eta(r) \in C_0^\infty(\mathbb{R})$ be a function such that $\eta(r) = r$ for $-1 < r < 1$ and $|\eta'(r)| \le 1$. For any $m \in \mathbb{N}$ we set $\rho_m(x) := m\eta(\langle x\rangle/m)$. By a direct calculation we have

$$\operatorname{Re}\langle(-\Delta\varphi_i^{k+1}), \rho_m^2\varphi_i^{k+1}\rangle = \|\nabla(\rho_m\varphi_i^{k+1})\|^2 - \|(\nabla\rho_m)\varphi_i^{k+1}\|^2.$$

Thus by (2.2) we obtain

(2.7)

$$\begin{aligned}
0 &= \operatorname{Re}\left\langle(-\Delta + V(x) + R^{\Phi^k}(x) - \epsilon_i^{k+1})\varphi_i^{k+1} - S^{\Phi^k}\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\right\rangle \\
&= \|\nabla(\rho_m\varphi_i^{k+1})\|^2 - \|(\nabla\rho_m)\varphi_i^{k+1}\|^2 \\
&\quad + \langle(V(x) + R^{\Phi^k}(x) - \epsilon_i^{k+1})\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle \\
&\quad - \operatorname{Re}\langle S^{\Phi^k}\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle \\
&\ge -\|(\nabla\rho_m)\varphi_i^{k+1}\|^2 + \langle(V(x) + R^{\Phi^k}(x) - \epsilon_i^{k+1})\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle \\
&\quad - \operatorname{Re}\langle S^{\Phi^k}\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle \\
&\ge -1 + \langle(V(x) + R^{\Phi^k}(x) - \epsilon_i^{k+1})\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle - \operatorname{Re}\langle S^{\Phi^k}\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle,
\end{aligned}$$

where we used $\|\varphi_i^{k+1}\| = 1$ and that $|\nabla\rho_m(z)| \le 1$ for any $z \in \mathbb{R}^3$.

Here we note that

$$|\rho_m(x) - \rho_m(y)| = \left|\int_0^1 (x-y)\cdot\nabla\rho_m(t(x-y)+y)dt\right| \le |x-y|.$$

Thus we have

$$\begin{aligned}
&|\langle S_{jj}^{\Phi^k}\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle - \langle S_{jj}^{\Phi^k}\rho_m\varphi_i^{k+1}, \rho_m\varphi_i^{k+1}\rangle| \\
&\quad = \left|\int |x-y|^{-1}\varphi_j^k(y)\overline{\varphi_i^{k+1}}(y)\rho_m(x)(\rho_m(x)-\rho_m(y))\overline{\varphi_j^k}(x)\varphi_i^{k+1}(x)dxdy\right| \\
&\quad \le \int \left|\varphi_j^k(y)\overline{\varphi_i^{k+1}}(y)\rho_m(x)\overline{\varphi_j^k}(x)\varphi_i^{k+1}(x)\right| dxdy \\
&\quad \le \||\rho_m|^{1/2}\varphi_j^k\|\||\rho_m|^{1/2}\varphi_i^{k+1}\|,
\end{aligned}$$

where $\overline{u}$ is the complex conjugate of u. Since the factors in the right-hand side are estimated as

$$\begin{aligned}
\||\rho_m|^{1/2}\varphi_i^{k+1}\| &= \left(\int |\rho_m(x)||\varphi_i^{k+1}(x)|^2dx\right)^{1/2} \\
&\le \|\rho_m\varphi_i^{k+1}\|^{1/2}\|\varphi_i^{k+1}\|^{1/2} = \|\rho_m\varphi_i^{k+1}\|^{1/2},
\end{aligned}$$

we obtain

$$\begin{aligned}
&|\langle S_{jj}^{\Phi^k}\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle - \langle S_{jj}^{\Phi^k}\rho_m\varphi_i^{k+1}, \rho_m\varphi_i^{k+1}\rangle| \\
&\quad \le \|\rho_m\varphi_j^k\|^{1/2}\|\rho_m\varphi_i^{k+1}\|^{1/2} \\
&\quad \le (2\gamma)^{-1}N + (2N)^{-1}\gamma\|\rho_m\varphi_j^k\|\|\rho_m\varphi_i^{k+1}\| \\
&\quad \le (2\gamma)^{-1}N + (4N)^{-1}\gamma\|\rho_m\varphi_j^k\|^2 + (4N)^{-1}\gamma\|\rho_m\varphi_i^{k+1}\|^2 \\
&\quad \le (2\gamma)^{-1}N + (4N)^{-1}\gamma C_k + (4N)^{-1}\gamma\|\rho_m\varphi_i^{k+1}\|^2,
\end{aligned}$$

where γ is the gap in the uniform well-posedness. Therefore, we have

$$\begin{aligned}
&|\langle S^{\Phi^k}\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle - \langle S^{\Phi^k}\rho_m\varphi_i^{k+1}, \rho_m\varphi_i^{k+1}\rangle| \\
&\quad \le (2\gamma)^{-1}N^2 + 4^{-1}\gamma C_k + 4^{-1}\gamma\|\rho_m\varphi_i^{k+1}\|^2.
\end{aligned}$$

Thus by (2.7) and $\langle w, (R^{\Phi^k} - S^{\Phi^k})w\rangle \ge 0$ with $w = \rho_m\varphi_i^{k+1}$ we obtain

$$\begin{aligned}
0 &\ge -1 - (2\gamma)^{-1}N^2 - 4^{-1}\gamma C_k - 4^{-1}\gamma\|\rho_m\varphi_i^{k+1}\|^2 \\
&\quad + \langle (V(x) - \epsilon_i^{k+1})\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle \qquad (2.8) \\
&\ge -1 - (2\gamma)^{-1}N^2 - 4^{-1}\gamma C_k + \langle (V(x) + (3/4)\gamma)\varphi_i^{k+1}, \rho_m^2\varphi_i^{k+1}\rangle,
\end{aligned}$$

where we used $\epsilon_i^{k+1} \le -\gamma$ of Lemma 8 in the second inequality.

Now let $r_0 > 0$ be a constant such that $|V(x)| < \frac{\gamma}{4}$ for $|x| > r_0$. Then decomposing the integral in (2.8) into those on $|x| \le r_0$ and $|x| > r_0$ we have

$$\begin{aligned}
&2^{-1}\gamma \int_{|x|>r_0} \rho_m^2(x)|\varphi_i^{k+1}(x)|^2 dx \\
&\quad \le 1 + (2\gamma)^{-1}N^2 + 4^{-1}\gamma C_k + \int_{|x|\le r_0} |V(x) + (3/4)\gamma|\, \rho_m^2(x)|\varphi_i^{k+1}(x)|^2 dx \\
&\quad \le 1 + (2\gamma)^{-1}N^2 + 4^{-1}\gamma C_k + (1 + r_0^2)\left(2\sum_l Z_l \|\nabla\varphi_i^{k+1}\| + (3/4)\gamma\right) \\
&\quad \le 1 + (2\gamma)^{-1}N^2 + 4^{-1}\gamma C_k + (1 + r_0^2)\left(2\sum_l Z_l \tilde{C}_b + (3/4)\gamma\right),
\end{aligned}$$

where we used $|\rho_m(x)| \le \langle x\rangle$ and the Hardy inequality in the second inequality, and $\tilde{C}_b$ is the constant in Remark 10. Hence Fatou's lemma yields

$$\begin{aligned}
\int_{|x|>r_0} \langle x\rangle^2|\varphi_i^{k+1}(x)|^2 dx &= \liminf_{m\to\infty} \int_{|x|>r_0} \rho_m^2(x)|\varphi_i^{k+1}(x)|^2 dx \\
&\le 2^{-1}C_k + \hat{C},
\end{aligned}$$

where $\hat{C} := 2\gamma^{-1}\{1+(2\gamma)^{-1}N^2+(1+r_0^2)(2\sum_l Z_l\tilde{C}_b+(3/4)\gamma)\}$ is independent of k. Therefore, noting that

$$\int_{|x|\le r_0} \langle x\rangle^2|\varphi_i^{k+1}(x)|^2 dx \le 1 + r_0^2,$$

we obtain

$$\|\langle x\rangle\varphi_i^{k+1}\|^2 = \int \langle x\rangle^2|\varphi_i^{k+1}(x)|^2 dx \le 2^{-1}C_k + \hat{C} + 1 + r_0^2.$$

Thus setting $\check{C} := \hat{C} + 1 + r_0^2$ we can choose $C_{k+1} = 2^{-1}C_k + \check{C}$ in (2.6) with k replaced by $k+1$. Then we can easily see that

$$C_k = 2^{-k}C_0 + \check{C}\sum_{j=0}^{k-1} 2^{-j} \le C_0 + 2\check{C},$$

for any $k \geq 1$. Therefore, we can choose $\mathcal{C} := (C_0 + 2\check{C})^{1/2}$ as the constant in (2.5), which completes the proof. $\square$

Proof of Proposition 5. We have only to prove that any subsequence of $\{(\Phi^k, \Phi^{k+1})\}$ contains a subsequence converging to a point in $\Gamma_{\gamma,\mu}$. Proposition 5 follows from this assertion as follows. Suppose $d((\Phi^k, \Phi^{k+1}), \Gamma_{\gamma,\mu})$ does not converge to 0 against the result of Proposition 5. Then we can choose a constant $\delta > 0$ and a subsequence $\{(\Phi^{k_j}, \Phi^{k_j+1})\}$ such that $d((\Phi^{k_j}, \Phi^{k_j+1}), \Gamma_{\gamma,\mu}) \geq \delta$ for any j, which contradicts the assertion above.

Step 1. First we shall prove that any subsequence $\{\Phi^{k_j}\}$ of $\{\Phi^k\}$ contains a convergent subsequence in $\bigoplus_{i=1}^N L^2(\mathbb{R}^3)$. A bounded subset B of $L^2(\mathbb{R}^m)$, $m \in \mathbb{N}$ is relatively compact if and only if $\int_{|x|>R} |f(x)|^2 dx \to 0$ and $\int_{|\xi|>R} |\mathscr{F} f(\xi)|^2 d\xi \to 0$ as $R \to \infty$ both uniformly for $f \in B$, where $\mathscr{F} f(\xi)$ is the Fourier transform of $f(x)$ (cf. [16, Theorem 3]). By Lemma 12 there exists a constant $\mathcal{C}$ such that $\|\langle x\rangle \varphi_i^{k_j}(x)\| \leq \mathcal{C}$, $1 \leq i \leq N$ for any k_j. It follows from Remark 10 also that $\||\xi|\mathscr{F}\varphi_i^{k_j}(\xi)\| \leq \tilde{C}_b$, $1 \leq i \leq N$ for any k_j. Hence $\{\Phi^{k_j}\}$ is relatively compact and contains a convergent subsequence.

By the same argument as above we can see that there exists a Cauchy subsequence of $\{\Phi^{k_j-1}\}$ in $\bigoplus_{i=1}^N L^2(\mathbb{R}^3)$. Hence we can extract a Cauchy subsequence of $\{(\Phi^{k_j-1}, \Phi^{k_j})\}$ in $(\bigoplus_{i=1}^N L^2(\mathbb{R}^3)) \oplus (\bigoplus_{i=1}^N L^2(\mathbb{R}^3))$, still denoted by $\{(\Phi^{k_j-1}, \Phi^{k_j})\}$. Since by Lemma 8 and Remark 10 we have $\mathbf{e}^k \in [\inf \sigma(h), -\gamma]^N$, we can further extract a subsequence so that $\mathbf{e}^{k_j}$ will be a Cauchy sequence. Then using the equation $\mathcal{F}(\Phi^{k_j-1})\varphi_i^{k_j} = \epsilon_i^{k_j}$, we can see that

(2.9)
$$\begin{aligned}
&\|h(\varphi_i^{k_{j_1}} - \varphi_i^{k_{j_2}})\| \\
&\quad \leq \|(\epsilon_i^{k_{j_1}} - R^{\Phi^{k_{j_1}-1}} + S^{\Phi^{k_{j_1}-1}})\varphi_i^{k_{j_1}} - (\epsilon_i^{k_{j_2}} - R^{\Phi^{k_{j_2}-1}} + S^{\Phi^{k_{j_2}-1}})\varphi_i^{k_{j_2}}\|.
\end{aligned}$$

Noting that by the Hardy inequality we have estimates as

$$\begin{aligned}
\left|\int |x-y|^{-1}(\varphi_i^{k_{j_1}-1} - \varphi_i^{k_{j_2}-1})^*(y)\varphi_i^{k_{j_1}}(y)dy\right| &\leq 2\|\varphi_i^{k_{j_1}-1} - \varphi_i^{k_{j_2}-1}\|\|\nabla\varphi_i^{k_{j_1}}\| \\
&\leq 2\tilde{C}_b\|\varphi_i^{k_{j_1}-1} - \varphi_i^{k_{j_2}-1}\|,
\end{aligned}$$

with the constant $\tilde{C}_b$ in Remark 10, it follows from (2.9) that there exists a constant $\hat{C}_1 > 0$ such that

$$\begin{aligned}&\|h(\varphi_i^{k_{j_1}} - \varphi_i^{k_{j_2}})\|\\&\quad\le \hat{C}_1(\|\Phi^{k_{j_1}} - \Phi^{k_{j_2}}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)} + \|\Phi^{k_{j_1}-1} - \Phi^{k_{j_2}-1}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)}\\&\qquad + |\mathbf{e}^{k_{j_1}} - \mathbf{e}^{k_{j_2}}|).\end{aligned}$$

Because V is Δ-bounded with a relative bound smaller than 1, Δ is h-bounded, and therefore, we can conclude that $\{\Phi^{k_j}\}$ is a Cauchy sequence in $\bigoplus_{i=1}^N H^2(\mathbb{R}^3)$.

Step 2. In the same way as above we can see that there exists a convergent subsequence of $\{\Phi^{k_j+1}\}$ in $\bigoplus_{i=1}^N H^2(\mathbb{R}^3)$. Besides there exists a convergent subsequence of $\{(\mathbf{e}^{k_j}, \mathbf{e}^{k_j+1})\}$. Hence we can extract a Cauchy subsequence of $\{(\Phi^{k_j}, \Phi^{k_j+1})\}$ in $(\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N H^2(\mathbb{R}^3))$, still denoted by $\{(\Phi^{k_j}, \Phi^{k_j+1})\}$, such that $\{(\mathbf{e}^{k_j}, \mathbf{e}^{k_j+1})\}$ also converges. Set

$$(\Phi^\infty, \tilde{\Phi}^\infty) := \lim_{j\to\infty}\{(\Phi^{k_j}, \Phi^{k_j+1})\},$$

where $\Phi^\infty = {}^t(\varphi_1^\infty, \ldots, \varphi_N^\infty)$, $\tilde{\Phi}^\infty = {}^t(\tilde{\varphi}_1^\infty, \ldots, \tilde{\varphi}_N^\infty)$ and

$$(\mathbf{e}^\infty, \tilde{\mathbf{e}}^\infty) := \lim_{j\to\infty}\{(\mathbf{e}^{k_j}, \mathbf{e}^{k_j+1})\},$$

where $\mathbf{e}^\infty = (\epsilon_1^\infty, \ldots, \epsilon_N^\infty)$, $\tilde{\mathbf{e}}^\infty = (\tilde{\epsilon}_1^\infty, \ldots, \tilde{\epsilon}_N^\infty)$. Taking the limits in $L^2(\mathbb{R}^3)$ of the both sides of

$$\mathcal{F}(\Phi^{k_j})\varphi_i^{k_j+1} = \epsilon_i^{k_j+1}\varphi_i^{k_j+1},$$

we obtain

$$\mathcal{F}(\Phi^\infty)\tilde{\varphi}_i^\infty = \tilde{\epsilon}_i^\infty\tilde{\varphi}_i^\infty. \tag{2.10}$$

In order to consider the convergence of the other equation

$$\mathcal{F}(\Phi^{k_j-1})\varphi_i^{k_j} = \epsilon_i^{k_j}\varphi_i^{k_j}, \tag{2.11}$$

we shall prove $\lim_{j\to\infty}\|\mathcal{F}(\Phi^{k_j+1})\varphi_i^{k_j} - \mathcal{F}(\Phi^{k_j-1})\varphi_i^{k_j}\| = \lim_{j\to\infty} \|\mathcal{G}(\Phi^{k_j+1})\varphi_i^{k_j} - \mathcal{G}(\Phi^{k_j-1})\varphi_i^{k_j}\| = 0$. Recall that $\mathcal{E}(\Phi^k, \Phi^{k+1})$ converges to

μ. Hence by Lemmas 6 and 7 for any $\delta > 0$ there exists j_0 such that for any $j \geq j_0$ with appropriate $N \times N$ unitary matrices $\check{A}^-_{k_j-1}, \check{A}^+_{k_j+1}$ we have

$$\begin{aligned}
&\|\check{A}^+_{k_j+1}\Phi^{k_j+1} - \check{A}^-_{k_j-1}\Phi^{k_j-1}\|^2_{\oplus_{i=1}^N L^2(\mathbb{R}^3)} \\
&\quad \leq \|D_{\Phi^{k_j+1}} - D_{\Phi^{k_j-1}}\|_2^2 \\
&\quad \leq 2\gamma^{-1}(\mathcal{E}(\Phi^{k_j-1}, \Phi^{k_j}) - \mathcal{E}(\Phi^{k_j}, \Phi^{k_j+1})) \leq \delta.
\end{aligned}$$

Note also that by Remark 10 there exists a constant $\hat{C}_2 > 0$ independent of j such that

$$\begin{aligned}
\|\check{A}^+_{k_j+1}\Phi^{k_j+1}\|_{\oplus_{i=1}^N H^1(\mathbb{R}^3)} &= \|\Phi^{k_j+1}\|_{\oplus_{i=1}^N H^1(\mathbb{R}^3)} \leq \hat{C}_2, \\
\|\check{A}^-_{k_j-1}\Phi^{k_j-1}\|_{\oplus_{i=1}^N H^1(\mathbb{R}^3)} &= \|\Phi^{k_j-1}\|_{\oplus_{i=1}^N H^1(\mathbb{R}^3)} \leq \hat{C}_2.
\end{aligned}$$

Thus it follows from Lemma 11 that there exists a constant $\hat{C}_3 > 0$ such that for $j \geq j_0$

$$\begin{aligned}
&\|\mathcal{G}(\Phi^{k_j+1})\varphi_i^{k_j} - \mathcal{G}(\Phi^{k_j-1})\varphi_i^{k_j}\| \\
&\quad = \|\mathcal{G}(\check{A}^+_{k_j+1}\Phi^{k_j+1})\varphi_i^{k_j} - \mathcal{G}(\check{A}^-_{k_j-1}\Phi^{k_j-1})\varphi_i^{k_j}\| \\
&\quad \leq \hat{C}_3\|\check{A}^+_{k_j+1}\Phi^{k_j+1} - \check{A}^-_{k_j-1}\Phi^{k_j-1}\|_{\oplus_{i=1}^N L^2(\mathbb{R}^3)} \leq \hat{C}_3\delta^{1/2}.
\end{aligned}$$

Since we can choose arbitrarily small δ, This implies

$$\lim_{j\to\infty}\|\mathcal{G}(\Phi^{k_j+1})\varphi_i^{k_j} - \mathcal{G}(\Phi^{k_j-1})\varphi_i^{k_j}\| = 0.$$

Thus we have $\lim_{j\to\infty}\mathcal{F}(\Phi^{k_j-1})\varphi_i^{k_j} = \lim_{j\to\infty}\mathcal{F}(\Phi^{k_j+1})\varphi_i^{k_j} = \mathcal{F}(\tilde{\Phi}^\infty)\varphi_i^\infty$ in $L^2(\mathbb{R}^3)$. Hence taking the limits in the both sides of (2.11) we obtain

$$\mathcal{F}(\tilde{\Phi}^\infty)\varphi_i^\infty = \epsilon_i^\infty\varphi_i^\infty. \tag{2.12}$$

The conditions $\mathcal{E}(\Phi^\infty, \tilde{\Phi}^\infty) = \mu$ and $\epsilon_i^\infty, \tilde{\epsilon}_i^\infty \leq -\gamma$ follow from the definition $\mu = \lim_{k\to\infty}\mathcal{E}(\Phi^k, \Phi^{k+1})$ and Lemma 8, and therefore, by (2.10) and (2.12) we have $(\Phi^\infty, \tilde{\Phi}^\infty) \in \Gamma_{\gamma,\mu}$, which completes the proof. □

3. Compactness of Critical Sets

Let $\Gamma_{\gamma,\mu}$ be the set defined at the beginning of Section 2.

Proposition 13. *For any $\gamma > 0$ and $\mu \in \mathbb{R}$, the set $\Gamma_{\gamma,\mu}$ is a compact subset of $(\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N H^2(\mathbb{R}^3))$.*

The proof of this lemma is similar to that of Proposition 5. Therefore, we prepare the corresponding decay estimate.

Lemma 14. *Let $\gamma > 0$ and $\mu \in \mathbb{R}$. Then there exists a constant C'_γ such that for any $(\Phi, \tilde{\Phi}) \in \Gamma_{\gamma,\mu}$ we have*

$$\|\langle x\rangle \Phi\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)}, \|\langle x\rangle \tilde{\Phi}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)} \le C'_\gamma.$$

Proof. By exactly the same way as (2.8) we obtain

$$\begin{aligned}0 \ge & -1 - (2\gamma)^{-1}N^2 - (4N)^{-1}\gamma \sum_{j=1}^N \|\rho_m \tilde{\varphi}_j\|^2 - 4^{-1}\gamma\|\rho_m \varphi_i\|^2 \\ & + \langle (V(x) - \epsilon_i)\varphi_i, \rho_m^2 \varphi_i\rangle, \quad 1 \le i \le N,\end{aligned}$$

and

$$\begin{aligned}0 \ge & -1 - (2\gamma)^{-1}N^2 - (4N)^{-1}\gamma \sum_{j=1}^N \|\rho_m \varphi_i\|^2 - 4^{-1}\gamma\|\rho_m \tilde{\varphi}_i\|^2 \\ & + \langle (V(x) - \tilde{\epsilon}_i)\tilde{\varphi}_i, \rho_m^2 \tilde{\varphi}_i\rangle, \quad 1 \le i \le N.\end{aligned}$$

Adding the both sides of the inequalities for $1 \le i \le N$ and noting that $\epsilon_i, \tilde{\epsilon}_i \le -\gamma$ we have

$$0 \ge -2N - \gamma^{-1}N^3 + \sum_{i=1}^N \langle (V(x) + \gamma/2)\varphi_i, \rho_m^2 \varphi_i\rangle + \sum_{i=1}^N \langle (V(x) + \gamma/2)\varphi_i, \rho_m^2 \varphi_i\rangle.$$

Let $r_1 > 0$ be a constant such that $|V(x)| \le \gamma/4$ for $|x| > r_1$. Decomposing the integral into those on $|x| \le r_1$ and $|x| > r_1$ we have

$$\begin{aligned}& 4^{-1}\gamma \sum_{i=1}^N \int_{|x|>r_1} \rho_m^2(x)(|\varphi_i(x)|^2 + |\tilde{\varphi}_i(x)|^2)dx \\ & \le 2N + \gamma^{-1}N^3 + \sum_{i=1}^N \int_{|x|\le r_1} \rho_m^2(x)(|V(x)| + \gamma/2)(|\varphi_i(x)|^2 + |\tilde{\varphi}_i(x)|^2)dx \\ & \le 2N + \gamma^{-1}N^3 + N(1 + r_1^2)\left(4\sum_l Z_l \tilde{C}_b + \gamma\right),\end{aligned}$$

where $\tilde{C}_b$ is the constant in Remark 10. Fatou's lemma yields

$$\begin{aligned}&4^{-1}\gamma\sum_{i=1}^{N}\int_{|x|>r_1}\langle x\rangle^2(|\varphi_i(x)|^2+|\tilde{\varphi}_i(x)|^2)dx\\&\quad\le 2N+\gamma^{-1}N^3+N(1+r_1^2)\left(4\sum_l Z_l\tilde{C}_b+\gamma\right).\end{aligned}$$

Noting that

$$\int_{|x|\le r_1}\langle x\rangle^2(|\varphi_i(x)|^2+|\tilde{\varphi}_i(x)|^2)dx\le 2(1+r_1^2),$$

we obtain

$$\begin{aligned}&\sum_{i=1}^{N}(\|\langle x\rangle\varphi_i\|^2+\|\langle x\rangle\tilde{\varphi}_i\|^2)\\&\quad\le 4\gamma^{-1}\left(2N+\gamma^{-1}N^3+N(1+r_1^2)\left(4\sum_l Z_l\tilde{C}_b+\gamma\right)\right)+2N(1+r_1^2).\end{aligned}$$

Thus if we set

$$\begin{aligned}C'_\gamma:=\Bigg\{&4\gamma^{-1}\left(2N+\gamma^{-1}N^3+N(1+r_1^2)\left(4\sum_l Z_l\tilde{C}_b+\gamma\right)\right)\\&+2N(1+r_1^2)\Bigg\}^{1/2},\end{aligned}$$

the result follows. □

Proof of Proposition 13. Let $\{(\Phi^k,\tilde{\Phi}^k)\}\subset\Gamma_{\gamma,\mu}$ be an arbitrary sequence in $\Gamma_{\gamma,\mu}$. Using Lemma 14 in the same way as in the proof of Proposition 5 we can see that there exists a subsequence $\{(\Phi^{k_j},\tilde{\Phi}^{k_j})\}$ of $\{(\Phi^k,\tilde{\Phi}^k)\}$ converging to a point $(\Phi^\infty,\tilde{\Phi}^\infty)$ in $(\bigoplus_{i=1}^N H^2(\mathbb{R}^3))\bigoplus(\bigoplus_{i=1}^N H^2(\mathbb{R}^3))$, and the associated orbital energies $\mathbf{e}^{k_j}$ and $\tilde{\mathbf{e}}^{k_j}$ converge to some $\mathbf{e}^\infty=(\epsilon_1^\infty,\dots,\epsilon_N^\infty)$ and $\tilde{\mathbf{e}}^\infty=(\tilde{\epsilon}_1^\infty,\dots,\tilde{\epsilon}_N^\infty)$ respectively. Taking the limits in the both sides of

$$\begin{aligned}\mathcal{F}(\tilde{\Phi}^{k_j})\varphi_i^{k_j}&=\epsilon_i^{k_j}\varphi_i^{k_j}\\ \mathcal{F}(\Phi^{k_j})\tilde{\varphi}_i^{k_j}&=\tilde{\epsilon}_i^{k_j}\tilde{\varphi}_i^{k_j}\end{aligned}\qquad 1\le i\le N,$$

we obtain

$$\begin{aligned}\mathcal{F}(\tilde{\Phi}^\infty)\varphi_i^\infty &= \epsilon_i^\infty\varphi_i^\infty \\ \mathcal{F}(\Phi^\infty)\tilde{\varphi}_i^\infty &= \tilde{\epsilon}_i^\infty\tilde{\varphi}_i^\infty\end{aligned} \qquad 1 \le i \le N.$$

Since $\mathcal{E}(\Phi^\infty, \tilde{\Phi}^\infty) = \mu$ and $\epsilon_i^\infty, \tilde{\epsilon}_i^\infty \le -\gamma,\ 1 \le i \le N$ obviously hold, we can see that $(\Phi^\infty, \tilde{\Phi}^\infty) \in \Gamma_{\gamma,\mu}$, which completes the proof. □

4. Fredholm Property of Fréchet Derivatives

In this section we prove that the Fréchet second derivatives of an auxiliary functional are decomposed into sums of an isomorphism and a compact operator. Denote by

$$\mathcal{X} := (\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus \mathbb{R}^N \bigoplus \mathbb{R}^N,$$

and

$$\mathcal{Z} := (\bigoplus_{i=1}^N L^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N L^2(\mathbb{R}^3)) \bigoplus \mathbb{R}^N \bigoplus \mathbb{R}^N,$$

the direct sums of Banach spaces regarding $\bigoplus_{i=1}^N H^2(\mathbb{R}^3)$ and $\bigoplus_{i=1}^N L^2(\mathbb{R}^3)$ as real Banach spaces with respect to multiplication by real numbers. Let us introduce an auxiliary functional. We define a functional $f : \mathcal{X} \to \mathbb{R}$ by

$$f(\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}}) := \mathcal{E}(\Phi, \tilde{\Phi}) - \sum_{i=1}^N \epsilon_i(\|\varphi_i\|^2 - 1) - \sum_{i=1}^N \tilde{\epsilon}_i(\|\tilde{\varphi}_i\|^2 - 1). \tag{4.1}$$

We also define a bilinear form $\langle\langle\cdot,\cdot\rangle\rangle$ on $\mathcal{X}$ and $\mathcal{Z}$ by

$$\begin{aligned}\langle\langle[\Phi^1, \tilde{\Phi}^1, \mathbf{e}^1, \tilde{\mathbf{e}}^1], [\Phi^2, \tilde{\Phi}^2, \mathbf{e}^2, \tilde{\mathbf{e}}^2]\rangle\rangle :=& 2\sum_{i=1}^N \mathrm{Re}\,\langle\varphi_i^1, \varphi_i^2\rangle + 2\sum_{i=1}^N \mathrm{Re}\,\langle\tilde{\varphi}_i^1, \tilde{\varphi}_i^2\rangle \\ &+ \sum_{i=1}^N \epsilon_i^1\epsilon_i^2 + \sum_{i=1}^N \tilde{\epsilon}_i^1\tilde{\epsilon}_i^2,\end{aligned}$$

for $[\Phi^1, \tilde{\Phi}^1, \mathbf{e}^1, \tilde{\mathbf{e}}^1] \in \mathcal{X}$ and $[\Phi^2, \tilde{\Phi}^2, \mathbf{e}^2, \tilde{\mathbf{e}}^2] \in \mathcal{Z}$. Then the Fréchet derivative of f is given by

$$df([\Phi^0, \tilde{\Phi}^0, \mathbf{e}^0, \tilde{\mathbf{e}}^0], [\Phi^1, \tilde{\Phi}^1, \mathbf{e}^1, \tilde{\mathbf{e}}^1]) = \langle\langle[\Phi^1, \tilde{\Phi}^1, \mathbf{e}^1, \tilde{\mathbf{e}}^1], F(\Phi^0, \tilde{\Phi}^0, \mathbf{e}^0, \tilde{\mathbf{e}}^0)\rangle\rangle,$$

where $F : \mathcal{X} \to \mathcal{Z}$ is defined by

$$\begin{aligned}
&F(\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}}) \\
&\quad = \big[{}^t(F_1(\Phi, \tilde{\Phi}, \mathbf{e}), \dots, F_N(\Phi, \tilde{\Phi}, \mathbf{e})), {}^t(F_1(\tilde{\Phi}, \Phi, \tilde{\mathbf{e}}), \dots, F_N(\tilde{\Phi}, \Phi, \tilde{\mathbf{e}})), \\
&\qquad (1 - \|\varphi_1\|^2, \dots, 1 - \|\varphi_N\|^2), (1 - \|\tilde{\varphi}_1\|^2, \dots, 1 - \|\tilde{\varphi}_N\|^2)\big].
\end{aligned}$$

Here $F_i : (\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus \mathbb{R}^N \to L^2(\mathbb{R}^3)$ is given by

$$F_i(\Phi, \tilde{\Phi}, \mathbf{e}) := \mathcal{F}(\tilde{\Phi})\varphi_i - \epsilon_i \varphi_i.$$

Lemma 15. *For any* $[\Phi', \tilde{\Phi}', \mathbf{e}', \tilde{\mathbf{e}}'] \in \mathcal{X}$ *satisfying* $\epsilon_i', \tilde{\epsilon}_i' < 0$, $1 \le i \le N$, *the Fréchet derivative* $F'(\Phi', \tilde{\Phi}', \mathbf{e}', \tilde{\mathbf{e}}')$ *of* $F(\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}})$ *at* $[\Phi', \tilde{\Phi}', \mathbf{e}', \tilde{\mathbf{e}}']$ *is written as*

$$F'(\Phi', \tilde{\Phi}', \mathbf{e}', \tilde{\mathbf{e}}') = L + M,$$

where $\mathbf{e}' = (\epsilon_1' \dots, \epsilon_N')$, $\tilde{\mathbf{e}}' = (\tilde{\epsilon}_1' \dots, \tilde{\epsilon}_N')$, L *is an isomorphism of* $\mathcal{X}$ *onto* $\mathcal{Z}$ *and* M *is a compact operator.*

Proof. By the assumption clearly there exists a constant $\epsilon > 0$ such that $\epsilon_i', \tilde{\epsilon}_i' \le -\epsilon$, $1 \le i \le N$. For a mapping $G(\Phi, \tilde{\Phi}) : (\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \to L^2(\mathbb{R}^3)$ we denote by $G'_{\varphi_i} = G'_{\varphi_i}(\Phi', \tilde{\Phi}') : H^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ the partial derivative

$$\begin{aligned}
&G'_{\varphi_i}(\Phi', \tilde{\Phi}')h \\
&\quad := \lim_{t \to 0} [G(\varphi_1' \dots, \varphi_i' + th, \dots, \varphi_N', \tilde{\Phi}') - G(\varphi_1' \dots, \varphi_i', \dots, \varphi_N', \tilde{\Phi}')]/t,
\end{aligned}$$

with respect to φ_i at $(\Phi', \tilde{\Phi}')$, where $\Phi' = {}^t(\varphi_1', \dots, \varphi_N')$, $\tilde{\Phi}' = {}^t(\tilde{\varphi}_1', \dots, \tilde{\varphi}_N')$. The partial derivative $G'_{\tilde{\varphi}_i} = G'_{\tilde{\varphi}_i}(\Phi', \tilde{\Phi}') : H^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ with respect to $\tilde{\varphi}_i$ at $(\Phi', \tilde{\Phi}')$ is defined in the same way. For fixed $\mathbf{e}'$ and $\tilde{\mathbf{e}}'$ we shall consider the Fréchet derivative of the mapping $\check{F}(\Phi, \tilde{\Phi}) : (\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \to (\bigoplus_{i=1}^N L^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N L^2(\mathbb{R}^3))$ given by

$$\begin{aligned}
&\check{F}(\Phi, \tilde{\Phi}) \\
&\quad := [{}^t(F_1(\Phi, \tilde{\Phi}, \mathbf{e}'), \dots, F_N(\Phi, \tilde{\Phi}, \mathbf{e}')), {}^t(F_1(\tilde{\Phi}, \Phi, \tilde{\mathbf{e}}'), \dots, F_N(\tilde{\Phi}, \Phi, \tilde{\mathbf{e}}'))].
\end{aligned}$$

The Fréchet derivative

$$\check{F}'(\Phi',\tilde{\Phi}') : (\bigoplus_{i=1}^{N} H^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^{N} H^2(\mathbb{R}^3)) \to (\bigoplus_{i=1}^{N} L^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^{N} L^2(\mathbb{R}^3)),$$

of $\check{F}$ at $(\Phi',\tilde{\Phi}')$ can be expressed as a $2N \times 2N$ matrix of operators from $H^2(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3)$ as

$$\check{F}'(\Phi',\tilde{\Phi}') = \begin{pmatrix} K(\tilde{\Phi}',\mathbf{e}') & T^{\Phi',\tilde{\Phi}'} \\ T^{\tilde{\Phi}',\Phi'} & K(\Phi',\tilde{\mathbf{e}}') \end{pmatrix}, \tag{4.2}$$

where $K(\tilde{\Phi}',\mathbf{e}')$ is a diagonal matrix defined by

$$K(\tilde{\Phi}',\mathbf{e}') := \operatorname{diag}[\mathcal{F}(\tilde{\Phi}') - \epsilon_1', \ldots, \mathcal{F}(\tilde{\Phi}') - \epsilon_N'],$$

and the $N \times N$ matrix $T^{\Phi',\tilde{\Phi}'}$ of operators is given by

$$T_{ij}^{\Phi',\tilde{\Phi}'} = [F_i(\Phi,\tilde{\Phi},\mathbf{e}')]'_{\tilde{\varphi}_j} = \hat{S}_{ij}^{\Phi',\tilde{\Phi}'} + \check{S}_{ij}^{\Phi',\tilde{\Phi}'} - Q_{ij}^{\Phi',\tilde{\Phi}'} - \check{S}_{ji}^{\tilde{\Phi}',\Phi'}.$$

Here

$$\begin{aligned}
(\hat{S}_{ij}^{\Phi',\tilde{\Phi}'} w)(x) &:= \left(\int |x-y|^{-1}\overline{\tilde{\varphi}_j'}(y)w(y)dy\right)\varphi_i'(x), \\
(\check{S}_{ij}^{\Phi',\tilde{\Phi}'} w)(x) &:= \left(\int |x-y|^{-1}\overline{w}(y)\tilde{\varphi}_j'(y)dy\right)\varphi_i'(x), \\
(Q_{ij}^{\Phi',\tilde{\Phi}'} w)(x) &:= \left(\int |x-y|^{-1}\overline{\tilde{\varphi}_j'}(y)\varphi_i'(y)dy\right)w(x).
\end{aligned}$$

Let us define the matrices $\hat{S}^{\Phi',\tilde{\Phi}'}$, $\check{S}^{\Phi',\tilde{\Phi}'}$ and $Q^{\Phi',\tilde{\Phi}'}$ by the matrix elements $\hat{S}_{ij}^{\Phi',\tilde{\Phi}'}$, $\check{S}_{ij}^{\Phi',\tilde{\Phi}'}$ and $Q_{ij}^{\Phi',\tilde{\Phi}'}$ respectively. We can rewrite (4.2) as

$$\check{F}'(\Phi',\tilde{\Phi}') = \mathcal{K} + \mathcal{T},$$

with

$$\mathcal{K} := \begin{pmatrix} K(\tilde{\Phi}',\mathbf{e}') & 0 \\ 0 & K(\Phi',\tilde{\mathbf{e}}') \end{pmatrix}, \ \mathcal{T} := \begin{pmatrix} 0 & T^{\Phi',\tilde{\Phi}'} \\ T^{\tilde{\Phi}',\Phi'} & 0 \end{pmatrix}.$$

The matrices $\hat{\mathcal{S}}$, $\check{\mathcal{S}}$ and $\mathcal{Q}$ are defined replacing $T^{\Phi',\tilde{\Phi}'}$ in $\mathcal{T}$ by $\hat{S}^{\Phi',\tilde{\Phi}'}$, $\check{S}^{\Phi',\tilde{\Phi}'}$ and $Q^{\Phi',\tilde{\Phi}'}$ respectively. Then we have

$$\mathcal{T} = \hat{\mathcal{S}} + \check{\mathcal{S}} - \mathcal{Q} - {}^t\check{\mathcal{S}}.$$

On the other hand $\mathcal{K}$ is decomposed as

$$\mathcal{K} = \mathcal{H} + \mathcal{R} - \mathcal{S},$$

where

$$\begin{aligned}
\mathcal{H} &:= \operatorname{diag}[h-\epsilon'_1,\ldots,h-\epsilon'_N,h-\tilde{\epsilon}'_1,\ldots,h-\tilde{\epsilon}'_N],\\
\mathcal{R} &:= \operatorname{diag}[R^{\tilde{\Phi}'},\ldots,R^{\tilde{\Phi}'},R^{\Phi'},\ldots,R^{\Phi'}],\\
\mathcal{S} &:= \operatorname{diag}[S^{\tilde{\Phi}'},\ldots,S^{\tilde{\Phi}'},S^{\Phi'},\ldots,S^{\Phi'}].
\end{aligned}$$

Since $S_{ii}^{\tilde{\Phi}'}$, $S_{ii}^{\Phi'}$, $\hat{S}_{ij}^{\Phi',\tilde{\Phi}'}$ and $\check{S}_{ij}^{\Phi',\tilde{\Phi}'}$ are integral operators of the Hilbert-Schmidt type, they are compact. Thus $\mathcal{S}$, $\hat{\mathcal{S}}$, $\check{\mathcal{S}}$ and ${}^t\check{\mathcal{S}}$ are compact operators.

We shall show that $\mathcal{R}-\mathcal{Q}$ is a positive definite operator as an operator on the Hilbert space $(\bigoplus_{i=1}^N L^2(\mathbb{R}^3))\bigoplus(\bigoplus_{i=1}^N L^2(\mathbb{R}^3))$. Set $W := {}^t(w_1,\ldots,w_N,\tilde{w}_1,\ldots,\tilde{w}_N) \in (\bigoplus_{i=1}^N L^2(\mathbb{R}^3))\bigoplus(\bigoplus_{i=1}^N L^2(\mathbb{R}^3))$. Then we have

$$\begin{aligned}
\langle W,(\mathcal{R}-\mathcal{Q})W\rangle &= \sum_{i=1}^N \langle w_i, R^{\tilde{\Phi}'} w_i\rangle + \sum_{i=1}^N \langle \tilde{w}_i, R^{\Phi'}\tilde{w}_i\rangle\\
&\quad - \sum_{i,j=1}^N \langle w_i, Q_{ij}^{\Phi',\tilde{\Phi}'}\tilde{w}_j\rangle - \sum_{i,j=1}^N \langle \tilde{w}_i, Q_{ij}^{\tilde{\Phi}',\Phi'} w_j\rangle\\
&= \sum_{i,j=1}^N \{\langle w_i, Q_{jj}^{\tilde{\Phi}'} w_i\rangle + \langle \tilde{w}_j, Q_{ii}^{\Phi'}\tilde{w}_j\rangle\\
&\quad - \langle w_i, Q_{ij}^{\Phi',\tilde{\Phi}'}\tilde{w}_j\rangle - \langle \tilde{w}_j, Q_{ji}^{\tilde{\Phi}',\Phi'} w_i\rangle\}.
\end{aligned} \tag{4.3}$$

On the other hand we have

$$\begin{aligned}
&\int |x-y|^{-1}|w_i(x)\tilde{\varphi}'_j(y)-\tilde{w}_j(x)\varphi'_i(y)|^2 dxdy\\
&= \langle w_i, Q_{jj}^{\tilde{\Phi}'} w_i\rangle + \langle \tilde{w}_j, Q_{ii}^{\Phi'}\tilde{w}_j\rangle - \langle w_i, Q_{ij}^{\Phi',\tilde{\Phi}'}\tilde{w}_j\rangle - \langle \tilde{w}_j, Q_{ji}^{\tilde{\Phi}',\Phi'} w_i\rangle.
\end{aligned} \tag{4.4}$$

Since the left-hand side is positive, the right-hand side is also positive. Therefore, comparing (4.3) with (4.4) we can see that $\mathcal{R} - \mathcal{Q}$ is a positive definite operator.

Next we shall consider $\mathcal{H}$. We denote the resolution of identity of h by $E(\lambda)$. Then we can decompose h as

$$h = hE(-\epsilon/2) + h(1 - E(-\epsilon/2)).$$

Thus $\mathcal{H}$ is decomposed as $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$, where

$$\begin{aligned}\mathcal{H}_1 :=& \operatorname{diag}[h(1 - E(-\epsilon/2)) - \epsilon'_1, \ldots, h(1 - E(-\epsilon/2)) - \epsilon'_N,\\ & h(1 - E(-\epsilon/2)) - \tilde{\epsilon}'_1, \ldots, h(1 - E(-\epsilon/2)) - \tilde{\epsilon}'_N],\end{aligned}$$

and

$$\mathcal{H}_2 := \operatorname{diag}[hE(-\epsilon/2), \ldots, hE(-\epsilon/2), hE(-\epsilon/2), \ldots, hE(-\epsilon/2)].$$

Since $\epsilon'_i, \tilde{\epsilon}'_i \leq -\epsilon$, $1 \leq i \leq N$ we have $h(1 - E(-\epsilon/2)) - \epsilon'_i \geq \epsilon/2$, and $h(1 - E(-\epsilon/2)) - \tilde{\epsilon}'_i \geq \epsilon/2$, so that $\mathcal{H}_1 \geq \epsilon/2$. As for $\mathcal{H}_2$, $\inf \sigma_{ess}(h) = 0$ implies that $hE(-\epsilon/2)$ is a compact operator. Thus $\mathcal{H}_2$ is a compact operator.

The Fréchet derivative $\check{F}'(\Phi', \tilde{\Phi}')$ is written as

$$\check{F}'(\Phi', \tilde{\Phi}') = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{R} - \mathcal{S} + \hat{\mathcal{S}} + \check{\mathcal{S}} - \mathcal{Q} - {}^t\check{\mathcal{S}} = \mathcal{L} + \mathcal{M},$$

where $\mathcal{L} := \mathcal{H}_1 + \mathcal{R} - \mathcal{Q}$ and $\mathcal{M} := \mathcal{H}_2 - \mathcal{S} + \hat{\mathcal{S}} + \check{\mathcal{S}} - {}^t\check{\mathcal{S}}$. Since $\mathcal{H}_1 \geq \epsilon/2$ and $\mathcal{R} - \mathcal{Q} \geq 0$, we have $\mathcal{L} \geq \epsilon/2$, and thus $\mathcal{L}$ is invertible. Since $\mathcal{L}$ can be regarded as a self-adjoint operator in $(\bigoplus_{i=1}^N L^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N L^2(\mathbb{R}^3))$, we can see that $\operatorname{Ran} \mathcal{L} = (\bigoplus_{i=1}^N L^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N L^2(\mathbb{R}^3))$ and it is an isomorphism of $(\bigoplus_{i=1}^N H^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N H^2(\mathbb{R}^3))$ onto $(\bigoplus_{i=1}^N L^2(\mathbb{R}^3)) \bigoplus (\bigoplus_{i=1}^N L^2(\mathbb{R}^3))$. Moreover, since each term in $\mathcal{M}$ is a compact operator, $\mathcal{M}$ is also a compact operator.

For fixed $\Phi', \tilde{\Phi}'$ we set

$$\hat{F}(\mathbf{e}, \tilde{\mathbf{e}}) := {}^t(F_1(\Phi', \tilde{\Phi}', \mathbf{e}), \ldots, F_N(\Phi', \tilde{\Phi}', \mathbf{e}), F_1(\tilde{\Phi}', \Phi', \tilde{\mathbf{e}}), \ldots, F_N(\tilde{\Phi}', \Phi', \tilde{\mathbf{e}})).$$

Then we obtain

$$
\begin{aligned}
&F'(\Phi', \tilde{\Phi}', \mathbf{e}', \tilde{\mathbf{e}}')[\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}}] \\
&\quad = [\check{F}'(\Phi', \tilde{\Phi}')[\Phi, \tilde{\Phi}] + \hat{F}'(\mathbf{e}', \tilde{\mathbf{e}}')[\mathbf{e}, \tilde{\mathbf{e}}], \\
&\qquad - 2\mathrm{Re}\,\langle \varphi_1, \varphi_1' \rangle, \ldots, -2\mathrm{Re}\,\langle \varphi_N, \varphi_N' \rangle, \\
&\qquad - 2\mathrm{Re}\,\langle \tilde{\varphi}_1, \tilde{\varphi}_1' \rangle, \ldots, -2\mathrm{Re}\,\langle \tilde{\varphi}_N, \tilde{\varphi}_N' \rangle] \\
&\quad = L[\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}}] + M[\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}}],
\end{aligned}
$$

where

$$
\begin{aligned}
&L[\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}}] := [\mathcal{L}[\Phi, \tilde{\Phi}], \mathbf{e}, \tilde{\mathbf{e}}], \\
&M[\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}}] \\
&\quad := [\mathcal{M}[\Phi, \tilde{\Phi}] - [\mathbf{e}\Phi', \tilde{\mathbf{e}}\tilde{\Phi}'], -2\mathrm{Re}\,\langle \varphi_1, \varphi_1' \rangle - \epsilon_1, \ldots, -2\mathrm{Re}\,\langle \varphi_N, \varphi_N' \rangle - \epsilon_N, \\
&\qquad - 2\mathrm{Re}\,\langle \tilde{\varphi}_1, \tilde{\varphi}_1' \rangle - \tilde{\epsilon}_1, \ldots, -2\mathrm{Re}\,\langle \tilde{\varphi}_N, \tilde{\varphi}_N' \rangle - \tilde{\epsilon}_N].
\end{aligned}
$$

Here $\mathbf{e}\Phi' := {}^t(\epsilon_1\varphi_1', \ldots, \epsilon_N\varphi_N')$. We can easily see that L is an isomorphism and M is a compact operator, which completes the proof. □

5. Łojasiewicz Inequality

The Łojasiewicz inequality for functionals that satisfy a certain condition is crucial for the proof of the convergence of SCF sequences. Let us denote by $\|\cdot\|_X$ the norm in a Banach space X.

DEFINITION 16. Let X and Y be real Banach spaces and O be an open subset of X. The mapping $F : O \to Y$ is said to be real-analytic on O if the following conditions are fulfilled:

(i) For each $x \in O$ there exist Fréchet derivatives of arbitrary orders $d^m F(x, \ldots)$.

(ii) For each $x \in O$ there exists $\delta > 0$ such that for any $h \in X$ satisfying $\|h\|_X < \delta$ one has

$$F(x + h) = \sum_{m=0}^{\infty} \frac{1}{m!} d^m F(x, h^m),$$

(the convergence being locally uniform and absolute), where $h^m := [h, \ldots, h]$ (m-times).

LEMMA 17. *Let Z be a real Hilbert space equipped with an inner product $\langle\langle\cdot,\cdot\rangle\rangle$ and a norm $\|\cdot\|_Z := \langle\langle\cdot,\cdot\rangle\rangle^{1/2}$. Let X be a dense subspace of Z and assume that X is a real Banach space with respect to another norm $\|\cdot\|_X$ such that $\|x\|_Z \le \|x\|_X$ for any $x \in X$. Moreover, let $f(x)$ be a real-analytic functional in X and x^c a critical point of $f(x)$. Suppose that there exists a real-analytic mapping $F(x) : X \to Z$ such that*

(f1) $df(x, y) = \langle\langle y, F(x)\rangle\rangle$,

(f2) $F'(x^c) = L + M$, *where L is an isomorphism of X onto Z and M is a compact operator.*

(f3) $F'(x^c)$ *is a selfadjoint operator with the domain X, when it is regarded as an operator in Z.*

Then there exist constants $\kappa > 0$, $\theta \in (0, 1/2]$ and a neighborhood $U(x^c)$ of x^c such that

$$|f(x) - f(x^c)|^{1-\theta} \le \kappa\|F(x)\|_Z, \tag{5.1}$$

for any $x \in U(x^c)$.

For the proof of Lemma 17 we need the following real-analytic version of the implicit function theorem.

LEMMA 18 ([6, Proposition 2.1] see also [7, Lemma 3R]). *Let X, Y, Z be real Banach spaces, $O \subset X \times Y$ an open set and $[x_0, y_0] \in O$. Let $F : O \to Z$ be a real-analytic mapping such that $[F'_y(x_0, y_0)]^{-1}$ exists and $F(x_0, y_0) = 0$. Then there exist a neighborhood $U(x_0)$ in X of the point x_0 and a neighborhood $U(y_0)$ in Y of the point y_0 such that $U(x_0) \times U(y_0) \subset O$ and there exists one and only one mapping $y : U(x_0) \to U(y_0)$ for which $F(x, y(x)) = 0$ on $U(x_0)$. Moreover, y is a real-analytic mapping on $U(x_0)$.*

PROOF OF LEMMA 17. Due to the decomposition $F'(x^c) = L + M$, $F'(x^c)$ is a Fredholm operator (see e.g. [2, Proof of Theorem 2.1]). Thus $X_1 := \mathrm{Ker}\,(F'(x^c))$ is finite-dimensional. Set $X_2 := X_1^{\perp} \cap X$, where $X_1^{\perp}$ is the orthogonal subspace of X_1 in Z. Then we have $X = X_1 \bigoplus X_2$. In addition, $F'(x^c)$ is an isomorphism of X_2 onto a closed subspace $\tilde{Z} := F'(x^c)(X_2)$ of Z. We write $x = [x_1, x_2]$, $x_i \in X_i$ $(i = 1, 2)$ correspondingly to the decomposition $X = X_1 \bigoplus X_2$. Let us denote the norm $\|\cdot\|_X$ restricted to X_2 by $\|\cdot\|_{X_2}$ and the norm $\|\cdot\|_Z$ restricted to $\tilde{Z}$ by $\|\cdot\|_{\tilde{Z}}$ with which X_2 and $\tilde{Z}$ are regarded as Banach spaces.

If $X_1 = \{0\}$, then by the open mapping theorem $F'(x^c)^{-1} : \tilde{Z} \to X$ is continuous, and therefore, there exists a constant $\check{C}_1 > 0$ such that

$$\|\tilde{x}\|_X = \|F'(x^c)^{-1}F'(x^c)\tilde{x}\|_X \leq \check{C}_1\|F'(x^c)\tilde{x}\|_{\tilde{Z}} = \check{C}_1\|F'(x^c)\tilde{x}\|_Z, \tag{5.2}$$

for any $\tilde{x} \in X$. Since by the definition of the Fréchet derivative and $F(x^c) = 0$ we have $F(x) = F(x^c) + F'(x^c)(x - x^c) + o(\|x - x^c\|_X) = F'(x^c)(x - x^c) + o(\|x - x^c\|_X)$, using (5.2) we can see that there exists a neighborhood $\hat{U}(x^c)$ of x^c and constants $0 < \tau < \check{C}_1^{-1}$, $\check{C}_2 > 0$ such that

$$\|F(x)\|_Z \geq \check{C}_1^{-1}\|x - x^c\|_X - \tau\|x - x^c\|_X \geq \check{C}_2\|x - x^c\|_X, \tag{5.3}$$

for any $x \in \hat{U}(x^c)$. On the other hand since x^c is a critical point of $f(x)$, by the Taylor formula (see e.g. [21, Theorem 4.A]) we have

$$f(x) = f(x^c) + \int_0^1 (1-t)d^2f(x^c + t(x - x^c), (x - x^c)^2)dt.$$

Hence we can see that there exists a constant $\check{C}_3 > 0$ such that

$$|f(x) - f(x^c)| \leq \check{C}_3\|x - x^c\|_X^2, \tag{5.4}$$

for any $x \in \hat{U}(x^c)$. From (5.4) and (5.3) it is seen that (5.1) holds with $U(x^c) = \hat{U}(x^c)$, $\kappa = \check{C}_2^{-1}\check{C}_3^{1/2}$ and $\theta = 1/2$ if $X_1 = \{0\}$.

If $X_1 \neq \{0\}$, applying Lemma 18 to $P_{\tilde{Z}} \circ F$ with $X = X_1$, $Y = X_2$ and $Z = \tilde{Z}$ it follows that there exists neighborhoods $\hat{U}(x_1^c)$ of x_1^c, $\hat{U}(x_2^c)$ of x_2^c and a real-analytic mapping $\omega : \hat{U}(x_1^c) \to \hat{U}(x_2^c)$ such that $x = [x_1, x_2] \in \hat{U}(x_1^c) \times \hat{U}(x_2^c)$ satisfies $P_{\tilde{Z}} \circ F(x) = 0$ if and only if $x_2 = \omega(x_1)$, where $P_{\tilde{Z}}$ is the orthogonal projection from Z onto $\tilde{Z}$. Moreover, since $F'(x^c)$ is selfadjoint, we have $X_1 = \mathrm{Ker}\,(F'(x^c)) = \mathrm{Ker}\,(F'(x^c)^*) = \tilde{Z}^\perp$. Let $\nu := \dim X_1$ and $\{v_1, \ldots, v_\nu\}$ be a basis of X_1. Set $\mathbf{v} := (v_1, \ldots, v_\nu)$. We write $\mathbf{t}\cdot\mathbf{v} := \sum_{j=1}^\nu t_jv_j$ for $\mathbf{t} = (t_1, \ldots, t_\nu) \in \mathbb{R}^\nu$. Then any $x_1 \in \hat{U}(x_1^c)$ is expressed as $x_1 = x_1^c + \mathbf{t}\cdot\mathbf{v}$, and $f(x_1^c + \mathbf{t}\cdot\mathbf{v}, \omega(x_1^c + \mathbf{t}\cdot\mathbf{v}))$ is a real-analytic function of $\mathbf{t} \in \mathbb{R}^\nu$ since f and ω are real-analytic. Thus applying the Łojasiewicz inequality in finite-dimensional space we can see that there exist constants

$\kappa_1, \kappa_2 > 0$, $\theta \in (0, 1/2]$ and a neighborhood $\check{U}(x_1^c)$ of x_1^c such that for any $x_1 \in U(x_1^c)$

$$\begin{aligned}
&|f(x_1,\omega(x_1)) - f(x_1^c,x_2^c)|^{1-\theta} \\
&\quad = |f(x_1,\omega(x_1)) - f(x_1^c,\omega(x_1^c))|^{1-\theta} \\
&\quad = |f(x_1^c + \mathbf{t}\cdot\mathbf{v}, \omega(x_1^c + \mathbf{t}\cdot\mathbf{v})) - f(x_1^c,\omega(x_1^c))|^{1-\theta} \\
&\quad = \kappa_1 \sum_{j=1}^{\nu} \Big| \{ \langle\langle v_j, F(x_1^c + \mathbf{t}\cdot\mathbf{v}, \omega(x_1^c + \mathbf{t}\cdot\mathbf{v}))\rangle\rangle \\
&\qquad + \langle\langle \omega'(x_1^c + \mathbf{t}\cdot\mathbf{v})[v_j], F(x_1^c + \mathbf{t}\cdot\mathbf{v}, \omega(x_1^c + \mathbf{t}\cdot\mathbf{v}))\rangle\rangle \} \Big| \\
&\quad \le \kappa_2 \|F(x_1^c + \mathbf{t}\cdot\mathbf{v}, \omega(x_1^c + \mathbf{t}\cdot\mathbf{v}))\|_Z \\
&\quad = \kappa_2 \|F(x_1,\omega(x_1))\|_Z,
\end{aligned} \tag{5.5}$$

where we used that $\|\omega'(x_1^c + \mathbf{t}\cdot\mathbf{v})[v_j]\|_Z \le \|\omega'(x_1^c + \mathbf{t}\cdot\mathbf{v})[v_j]\|_X \le C$ for a constant $C > 0$ independent of $\mathbf{t}$ such that $x_1^c + \mathbf{t}\cdot\mathbf{v} \in \check{U}(x_1^c)$.

By the open mapping theorem $[P_{\tilde{Z}} F'_{x_2}(x_1^c, x_2^c)]^{-1} : \tilde{Z} \to X_2$ is continuous. Thus there exists a constant $\check{C}_4 > 0$ such that

$$\begin{aligned}
\|\tilde{x}_2\|_{X_2} &= \|[P_{\tilde{Z}} F'_{x_2}(x_1^c, x_2^c)]^{-1} P_{\tilde{Z}} F'_{x_2}(x_1^c, x_2^c)\tilde{x}_2\|_{X_2} \\
&\le \check{C}_4 \|P_{\tilde{Z}} F'_{x_2}(x_1^c, x_2^c)\tilde{x}_2\|_{\tilde{Z}} = \check{C}_4 \|P_{\tilde{Z}} F'_{x_2}(x_1^c, x_2^c)\tilde{x}_2\|_Z,
\end{aligned} \tag{5.6}$$

for any $\tilde{x}_2 \in X_2$. Since $F(x)$ is a real-analytic mapping, choosing $\hat{U}(x_1^c)$ and $\hat{U}(x_2^c)$ small enough and using (5.6) we can see that there exists $\check{C}_5 > 0$ such that

$$\begin{aligned}
&\|P_{\tilde{Z}} F'_{x_2}(x_1,\omega(x_1))\tilde{x}_2\|_Z \\
&\quad \ge \|P_{\tilde{Z}} F'_{x_2}(x_1^c, x_2^c)\tilde{x}_2\|_Z - \|(P_{\tilde{Z}} F'_{x_2}(x_1,\omega(x_1)) - P_{\tilde{Z}} F'_{x_2}(x_1^c, x_2^c))\tilde{x}_2\|_Z \\
&\quad \ge \check{C}_5 \|\tilde{x}_2\|_{X_2},
\end{aligned} \tag{5.7}$$

for any $x_1 \in \hat{U}(x_1^c)$ and $\tilde{x}_2 \in X_2$. Moreover, by the definition of the Fréchet derivative and $P_{\tilde{Z}} F(x_1, \omega(x_1)) = 0$ we have

$$\begin{aligned}
&P_{\tilde{Z}} F(x_1, x_2) \\
&\quad = P_{\tilde{Z}} F(x_1,\omega(x_1)) + P_{\tilde{Z}} F'_{x_2}(x_1,\omega(x_1))(x_2 - \omega(x_1)) + o(\|x_2 - \omega(x_1)\|_{X_2}) \\
&\quad = P_{\tilde{Z}} F'_{x_2}(x_1,\omega(x_1))(x_2 - \omega(x_1)) + o(\|x_2 - \omega(x_1)\|_{X_2}),
\end{aligned} \tag{5.8}$$

for any $x_1 \in \hat{U}(x_1^c)$ and $x_2 \in \hat{U}(x_2^c)$. It follows from (5.7) and (5.8) that choosing smaller $\hat{U}(x_1^c)$ and $\hat{U}(x_2^c)$ further there exists $\check{C}_6 > 0$ such that

$$\|P_{\tilde{Z}} F(x_1, x_2)\|_Z \geq \check{C}_6 \|x_2 - \omega(x_1)\|_{X_2}, \tag{5.9}$$

for any $x_1 \in \hat{U}(x_1^c)$ and $x_2 \in \hat{U}(x_2^c)$. Moreover, using (5.9) we can see that there exists $\check{C}_7 > 0$ such that

$$\begin{aligned} \|F(x_1, \omega(x_1))\|_Z &\leq \|F(x_1, x_2)\|_Z + \|F(x_1, x_2) - F(x_1, \omega(x_1))\|_Z \\ &\leq \|F(x_1, x_2)\|_Z + \check{C}_7 \|x_2 - \omega(x_1)\|_Z \\ &\leq (1 + \check{C}_7 \check{C}_6^{-1}) \|F(x_1, x_2)\|_Z. \end{aligned} \tag{5.10}$$

On the other hand, since $P_{\tilde{Z}} F(x_1, \omega(x_1)) = 0$, we have

$$\begin{aligned} &f(x_1, x_2) - f(x_1, \omega(x_1)) \\ &\quad = \langle\langle x_2 - \omega(x_1), P_{\tilde{Z}^\perp} F(x_1, \omega(x_1))\rangle\rangle + O(\|x_2 - \omega(x_1)\|_{X_2}^2), \end{aligned}$$

where $P_{\tilde{Z}^\perp}$ is the orthogonal projection onto $\tilde{Z}^\perp$. Since $\tilde{Z}^\perp = X_1$ and $X_1 \perp X_2$ with respect to the inner product $\langle\langle \cdot, \cdot \rangle\rangle$ in Z, the first term in the right-hand side vanishes. Thus there exists a constant $\check{C}_8 > 0$ such that

$$|f(x_1, x_2) - f(x_1, \omega(x_1))| \leq \check{C}_8 \|x_2 - \omega(x_1)\|_{X_2}^2, \tag{5.11}$$

for any $x_1 \in \hat{U}(x_1^c)$ and $x_2 \in \hat{U}(x_2^c)$. Combining (5.9) and (5.11) we obtain

$$|f(x_1, x_2) - f(x_1, \omega(x_1))|^{1/2} \leq \check{C}_6^{-1} \check{C}_8^{1/2} \|F(x_1, x_2)\|_Z.$$

It follows from (5.5), (5.10) and (5.11) that for $x \in U(x^c) := (\check{U}(x_1^c) \cap \hat{U}(x_1^c)) \times \hat{U}(x_2^c)$ we have

$$\begin{aligned} &|f(x_1, x_2) - f(x^c)|^{1-\theta} \\ &\quad = |f(x_1, x_2) - f(x_1, \omega(x_1)) + f(x_1, \omega(x_1)) - f(x^c)|^{1-\theta} \\ &\quad \leq 2^{1-\theta} (|f(x_1, x_2) - f(x_1, \omega(x_1))|^{1-\theta} + |f(x_1, \omega(x_1)) - f(x^c)|^{1-\theta}) \\ &\quad \leq 2^{1-\theta} (|f(x_1, x_2) - f(x_1, \omega(x_1))|^{1/2} + |f(x_1, \omega(x_1)) - f(x^c)|^{1-\theta}) \\ &\quad \leq 2^{1-\theta} (\check{C}_6^{-1} \check{C}_8^{1/2} + \kappa_2 (1 + \check{C}_7 \check{C}_6^{-1})) \|F(x_1, x_2)\|_Z, \end{aligned}$$

where in the third step we assume $|f(x_1, x_2) - f(x_1, \omega(x_1))| < 1$, which holds if we choose sufficiently small $U(x^c)$. Thus (5.1) holds with $\kappa = 2^{1-\theta} (\check{C}_6^{-1} \check{C}_8^{1/2} + \kappa_2 (1 + \check{C}_7 \check{C}_6^{-1}))$, which completes the proof. □

6. Proof of the Main Theorems

For the proof of Theorem 1 the following lemma about convergence of positive term series is needed.

LEMMA 19. *Let* $(\alpha_1, \alpha_2, \dots)$ *be a sequence of real numbers such that* $\alpha_k > 0$ *for any* $k \geq 1$ *and* $\sum_{k=1}^{\infty} \frac{\alpha_{k+1}^2}{\alpha_k}$ *converges. Then* $\sum_{k=1}^{\infty} \alpha_k$ *converges.*

PROOF. Let $k_0 \in \mathbb{N}$ be a fixed number. Then by the Cauchy-Schwarz inequality we have

$$\sum_{k=1}^{k_0} \alpha_{k+1} = \sum_{k=1}^{k_0} \frac{\alpha_{k+1}}{\alpha_k^{1/2}} \alpha_k^{1/2} \leq \left(\sum_{k=1}^{k_0} \frac{\alpha_{k+1}^2}{\alpha_k} \right)^{1/2} \left(\sum_{k=1}^{k_0} \alpha_k \right)^{1/2}.$$

Hence we have

$$\sum_{k=1}^{k_0} \alpha_k \leq \alpha_1 + \sum_{k=1}^{k_0} \alpha_{k+1} \leq \alpha_1 + \left(\sum_{k=1}^{k_0} \frac{\alpha_{k+1}^2}{\alpha_k} \right)^{1/2} \left(\sum_{k=1}^{k_0} \alpha_k \right)^{1/2}.$$

Dividing both sides by $\left(\sum_{k=1}^{k_0} \alpha_k \right)^{1/2}$ we obtain

$$\left(\sum_{k=1}^{k_0} \alpha_k \right)^{1/2} \leq \alpha_1 \left(\sum_{k=1}^{k_0} \alpha_k \right)^{-1/2} + \left(\sum_{k=1}^{k_0} \frac{\alpha_{k+1}^2}{\alpha_k} \right)^{1/2} \leq \alpha_1^{1/2} + \left(\sum_{k=1}^{k_0} \frac{\alpha_{k+1}^2}{\alpha_k} \right)^{1/2}.$$

Since $\sum_{k=1}^{\infty} \frac{\alpha_{k+1}^2}{\alpha_k}$ converges, the right-hand side is bounded by a constant $C > 0$ independent of k_0, and therefore, we have

$$\sum_{k=1}^{k_0} \alpha_k \leq C^2.$$

Since k_0 was arbitrary, this implies that $\sum_{k=1}^{\infty} \alpha_k$ is convergent and

$$\sum_{k=1}^{\infty} \alpha_k \leq C^2,$$

which completes the proof. □

We also need a bound of the H^2 norm of differences of solutions to a sequence of equations by the L^2 norm.

Lemma 20. *Let $\zeta > 0$ be a constant and $\Xi^k = {}^t(\xi_1^k, \dots, \xi_N^k) \in \mathcal{W}$, $k = 0, 1, \dots$ be a sequence satisfying*

$$\mathcal{F}(\Xi^{k-1})\xi_i^k = \sum_{j=1}^N \epsilon_{ij}^k \xi_j^k,$$

with some constants ϵ_{ij}^k, $1 \le i, j \le N$ such that $|\epsilon_{ij}^k| \le \zeta$, $1 \le i, j \le N$ for any $k \ge 1$. Then there exists a constant $\beta_\zeta > 0$ independent of k such that

$$\begin{aligned}&\|\Xi^{k+1} - \Xi^{k-1}\|_{\oplus_{i=1}^N H^2(\mathbb{R}^3)} \\ &\quad \le \beta_\zeta(\|\Xi^k - \Xi^{k-2}\|_{\oplus_{i=1}^N L^2(\mathbb{R}^3)} + \|\Xi^{k+1} - \Xi^{k-1}\|_{\oplus_{i=1}^N L^2(\mathbb{R}^3)}),\end{aligned}$$

for any $k \ge 2$.

Proof. First note that by the same proof as that of Lemma 9 we can see that there exists a constant $\tilde{C}'_\zeta > 0$ such that

$$\|\nabla \xi_i^k\| \le \tilde{C}'_\zeta, \ 1 \le i \le N, \tag{6.1}$$

for any $k \ge 0$. It follows from the equations

$$\begin{aligned}\mathcal{F}(\Xi^{k-2})\xi_i^{k-1} &= \sum_{j=1}^N \epsilon_{ij}^{k-1}\xi_j^{k-1}, \\ \mathcal{F}(\Xi^{k})\xi_i^{k+1} &= \sum_{j=1}^N \epsilon_{ij}^{k+1}\xi_j^{k+1},\end{aligned} \tag{6.2}$$

(6.1) and Lemma 11 that there exists a constant $\tilde{\beta}_\zeta > 0$ independent of k such that

$$\begin{aligned}&\|h(\xi_i^{k+1} - \xi_i^{k-1})\| \\ &\quad = \|\mathcal{G}(\Xi^k)\xi_i^{k+1} - \sum_{j=1}^N \epsilon_{ij}^{k+1}\xi_j^{k+1} - \mathcal{G}(\Xi^{k-2})\xi_i^{k-1} + \sum_{j=1}^N \epsilon_{ij}^{k-1}\xi_j^{k-1}\| \\ &\quad \le \tilde{\beta}_\zeta(\|\Xi^k - \Xi^{k-2}\|_{\oplus_{i=1}^N L^2(\mathbb{R}^3)} + \|\Xi^{k+1} - \Xi^{k-1}\|_{\oplus_{i=1}^N L^2(\mathbb{R}^3)} \\ &\qquad + \sum_{j=1}^N |\epsilon_{ij}^{k+1} - \epsilon_{ij}^{k-1}|).\end{aligned} \tag{6.3}$$

By (6.2) we have

$$\epsilon_{ij}^{k-1} = \langle \xi_j^{k-1}, \mathcal{F}(\Xi^{k-2})\xi_i^{k-1} \rangle,$$
$$\epsilon_{ij}^{k+1} = \langle \xi_j^{k+1}, \mathcal{F}(\Xi^{k})\xi_i^{k+1} \rangle.$$

Thus by (6.1) and Lemma 11 there exists a constant $\hat{\beta}_\zeta > 0$ independent of k such that

$$\begin{aligned}|\epsilon_{ij}^{k+1} - \epsilon_{ij}^{k-1}| \leq \hat{\beta}_\zeta(&\|\Xi^k - \Xi^{k-2}\|_{\oplus_{i=1}^{N} L^2(\mathbb{R}^3)} \\ &+ \|\xi_i^{k+1} - \xi_i^{k-1}\| + \|\xi_j^{k+1} - \xi_j^{k-1}\|).\end{aligned} \tag{6.4}$$

Since Δ is h-bounded, the result immediately follows from (6.3) and (6.4). □

Proof of the Theorem 1. *Step* 1. First note that if $\|D_{\Phi^{k+1}} - D_{\Phi^{k-1}}\|_2 = 0$ for some k, then $\mathcal{F}(\Phi^{k+1}) = \mathcal{F}(\Phi^{k-1})$, and thus $D_{\Phi^{k+2}} = D_{\Phi^k}$. Therefore, by induction we have $D_{\Phi^s} = D_{\Phi^{s+2}}$ for any $s \geq k$. Then since Φ^{k+2t}, $t = 0, 1, \dots$ (resp., Φ^{k+2t+1}, $t = 0, 1, \dots$) are tuples of the eigenfunctions corresponding to the same eigenvalues of $\mathcal{F}(\Phi^{k-1})$ (resp., $\mathcal{F}(\Phi^k)$), there exist unitary matrices A_{k+2t} (resp., A_{k+2t+1}) such that $\|A_{k+2t}\Phi^{k+2t} - \Phi^k\| = 0$ (resp., $\|A_{k+2t+1}\Phi^{k+2t+1} - \Phi^{k+1}\| = 0$) for $t \geq 0$. Hence the results in Theorem 1 are obvious in this case. Therefore, hereafter we assume $\|D_{\Phi^{k+1}} - D_{\Phi^{k-1}}\|_2 > 0$ for any $k \geq 1$. As in Section 2, $\mathcal{E}(\Phi^k, \Phi^{k+1})$ is decreasing with respect to k and converges to some $\mu \in \mathbb{R}$. If $\mathcal{E}(\Phi^k, \Phi^{k+1}) = \mu$ for some k, then we have $\mu = \mathcal{E}(\Phi^k, \Phi^{k+1}) \geq \mathcal{E}(\Phi^{k+1}, \Phi^{k+2}) \geq \mu$, and therefore, $\mathcal{E}(\Phi^k, \Phi^{k+1}) = \mathcal{E}(\Phi^{k+1}, \Phi^{k+2})$. Recalling that by Lemma 6 we have

$$\mathcal{E}(\Phi^k, \Phi^{k+1}) - \mathcal{E}(\Phi^{k+1}, \Phi^{k+2}) \geq 2^{-1}\gamma\|D_{\Phi^{k+2}} - D_{\Phi^k}\|_2^2, \tag{6.5}$$

we obtain $\|D_{\Phi^{k+2}} - D_{\Phi^k}\|_2 = 0$, which contradicts the assumption above. Thus we may also assume $\mathcal{E}(\Phi^k, \Phi^{k+1}) > \mu$ for any $k \geq 0$.

We can easily see that for any constants $p \geq q > 0$ and $\tilde{\theta} \in (0, 1/2]$ we have

$$p^{\tilde{\theta}} - q^{\tilde{\theta}} \geq \frac{\tilde{\theta}}{p^{1-\tilde{\theta}}}(p - q).$$

Applying this inequality to $p = \mathcal{E}(\Phi^k, \Phi^{k+1}) - \mu$, $q = \mathcal{E}(\Phi^{k+1}, \Phi^{k+2}) - \mu$ we obtain

$$(6.6)\qquad \begin{aligned}&(\mathcal{E}(\Phi^k,\Phi^{k+1})-\mu)^{\tilde\theta}-(\mathcal{E}(\Phi^{k+1},\Phi^{k+2})-\mu)^{\tilde\theta}\\ &\geq \frac{\tilde\theta}{(\mathcal{E}(\Phi^k,\Phi^{k+1})-\mu)^{1-\tilde\theta}}(\mathcal{E}(\Phi^k,\Phi^{k+1})-\mathcal{E}(\Phi^{k+1},\Phi^{k+2})).\end{aligned}$$

The factor $(\mathcal{E}(\Phi^k,\Phi^{k+1})-\mathcal{E}(\Phi^{k+1},\Phi^{k+2}))$ in the right-hand side is estimated from below by (6.5).

Step 2. As for the denominator in the right-hand side of (6.6), recalling $\|\varphi_i^k\|, \|\varphi_i^{k+1}\|=1$, $1\leq i\leq N$ we can see that

$$(6.7)\qquad \mathcal{E}(\Phi^k,\Phi^{k+1})=f(\Phi^k,\Phi^{k+1},\mathbf{e}^k,\mathbf{e}^{k+1}),$$

where f is the functional defined by (4.1). Set

$$\tilde\Gamma_{\gamma,\mu}:=\{[\Phi,\tilde\Phi,\mathbf{e},\tilde{\mathbf{e}}]:[\Phi,\tilde\Phi]\in\Gamma_{\gamma,\mu},\ \epsilon_i:=\langle\varphi_i,\mathcal{F}(\tilde\Phi)\varphi_i\rangle,\ \tilde\epsilon_i:=\langle\tilde\varphi_i,\mathcal{F}(\Phi)\tilde\varphi_i\rangle\},$$

and let $\tilde d$ be the distance function in $(\bigoplus_{i=1}^N H^2(\mathbb{R}^3))\bigoplus(\bigoplus_{i=1}^N H^2(\mathbb{R}^3))\bigoplus\mathbb{R}^N\bigoplus\mathbb{R}^N$. As in the proof of Proposition 5 using Lemmas 6 and 7 we can show

$$(6.8)\qquad \lim_{k\to\infty}|\langle\varphi_i^k,\mathcal{F}(\Phi^{k+1})\varphi_i^k\rangle-\langle\varphi_i^k,\mathcal{F}(\Phi^{k-1})\varphi_i^k\rangle|=0.$$

Using Lemma 5, $\epsilon_i^k=\langle\varphi_i^k,\mathcal{F}(\Phi^{k-1})\varphi_i^k\rangle$ and (6.8) we can see that

$$(6.9)\qquad \lim_{k\to\infty}\tilde d([\Phi^k,\Phi^{k+1},\mathbf{e}^k,\mathbf{e}^{k+1}],\tilde\Gamma_{\gamma,\mu})=0.$$

By Lemma 15 for any $[\Phi',\tilde\Phi',\mathbf{e}',\tilde{\mathbf{e}}']\in\tilde\Gamma_{\gamma,\mu}$, $F'(\Phi',\tilde\Phi',\mathbf{e}',\tilde{\mathbf{e}}')$ is decomposed into a sum of an isomorphism L and a compact operator M. Moreover, extending the domain of $\langle\langle\cdot,\cdot\rangle\rangle$ from $\mathcal{X}\times\mathcal{Z}$ to $\mathcal{Z}\times\mathcal{Z}$ in the obvious way, $\mathcal{Z}$ can be regarded as a real Hilbert space equipped with the inner product $\langle\langle\cdot,\cdot\rangle\rangle$. Since the Fréchet derivative is symmetric [21, Problem 4.3], we have $d^2f(z_1,[z_2,z_3])=d^2f(z_1,[z_3,z_2])=\langle\langle z_2,F'(z_1)z_3\rangle\rangle=\langle\langle z_3,F'(z_1)z_2\rangle\rangle=\langle\langle F'(z_1)z_2,z_3\rangle\rangle$ for any $z_1,z_2,z_3\in\mathcal{X}$. Thus $F'(z_1)$ is a symmetric operator with the domain $\mathcal{X}\subset\mathcal{Z}$. The operator $F'(z_1)$ is a sum of $\tilde{\mathcal{H}}:=\operatorname{diag}[h,\dots,h,0,\dots,0]$ (h appears $2N$ times) and a bounded operator, and $\tilde{\mathcal{H}}$ is a selfadjoint operator with the domain $\mathcal{X}$ in the real Hilbert space $\mathcal{Z}$ equipped with the inner product $\langle\langle\cdot,\cdot\rangle\rangle$, which follows from that h is a selfadjoint operator with the domain $H^2(\mathbb{R}^3)$ in $L^2(\mathbb{R}^3)$ equipped with the usual inner product. Thus $F'(z_1)$ is also a selfadjoint operator with the domain $\mathcal{X}$. It is also easily seen that f and F are real-analytic. Therefore, we can apply Lemma 17 to f and see that there exist a neighborhood U of $[\Phi', \tilde{\Phi}', \mathbf{e}', \tilde{\mathbf{e}}']$ and constants $\kappa > 0$ and $\theta \in (0, 1/2]$ such that

$$|f(\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}}) - \mu|^{1-\theta} \leq \kappa \|F(\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}})\|_{\mathcal{Z}},$$

for any $[\Phi, \tilde{\Phi}, \mathbf{e}, \tilde{\mathbf{e}}] \in U$. Because by Proposition 13 $\Gamma_{\gamma,\mu}$ and therefore, $\tilde{\Gamma}_{\gamma,\mu}$ are compact, we can choose a finite cover of $\tilde{\Gamma}_{\gamma,\mu}$ from such neighborhoods. Therefore, by (6.9) there exist $\tilde{\kappa} > 0$, $\tilde{\theta} \in (0, 1/2]$ and $k_1 \in \mathbb{N}$ such that

$$|f(\Phi^k, \Phi^{k+1}, \mathbf{e}^k, \mathbf{e}^{k+1}) - \mu|^{1-\tilde{\theta}} \leq \tilde{\kappa} \|F(\Phi^k, \Phi^{k+1}, \mathbf{e}^k, \mathbf{e}^{k+1})\|_{\mathcal{Z}}, \tag{6.10}$$

for any $k \geq k_1$. Since $\|\varphi_i^k\|, \|\varphi_i^{k+1}\| = 1$, $1 \leq i \leq N$ and $\mathcal{F}(\Phi^k)\varphi_i^{k+1} = \epsilon_i^{k+1}\varphi_i^{k+1}$, $1 \leq i \leq N$, we can see that the $\mathbb{R}^N \bigoplus \mathbb{R}^N$ component and the second $\bigoplus_{i=1}^N L^2(\mathbb{R}^3)$ component of $F(\Phi^k, \Phi^{k+1}, \mathbf{e}^k, \mathbf{e}^{k+1})$ vanish. Thus we have

$$\|F(\Phi^k, \Phi^{k+1}, \mathbf{e}^k, \mathbf{e}^{k+1})\|_{\mathcal{Z}} = \left(\sum_{i=1}^N \|\mathcal{F}(\Phi^{k+1})\varphi_i^k - \epsilon_i^k \varphi_i^k\|_{L^2(\mathbb{R}^3)}^2\right)^{1/2}.$$

Using $\mathcal{F}(\Phi^{k-1})\varphi_i^k = \epsilon_i^k \varphi_i^k$ we obtain

(6.11)

$$\begin{aligned}\|F(\Phi^k, \Phi^{k+1}, \mathbf{e}^k, \mathbf{e}^{k+1})\|_{\mathcal{Z}} &= \left(\sum_{i=1}^N \|\mathcal{F}(\Phi^{k+1})\varphi_i^k - \mathcal{F}(\Phi^{k-1})\varphi_i^k\|_{L^2(\mathbb{R}^3)}^2\right)^{1/2} \\ &= \left(\sum_{i=1}^N \|\mathcal{G}(\Phi^{k+1}) - \mathcal{G}(\Phi^{k-1}))\varphi_i^k\|_{L^2(\mathbb{R}^3)}^2\right)^{1/2}.\end{aligned}$$

Let us denote by A_{k+1}^+, A_{k-1}^- the $N \times N$ unitary matrices A and $\tilde{A}$ in Lemma 7 with Φ and $\tilde{\Phi}$ replaced by Φ^{k+1} and Φ^{k-1} respectively, namely we have

$$\begin{aligned}\|D_{\Phi^{k+1}} - D_{\Phi^{k-1}}\|_2 &\geq \|A_{k+1}^+ \Phi^{k+1} - A_{k-1}^- \Phi^{k-1}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)} \\ &= \|\tilde{\Xi}_+^{k+1} - \tilde{\Xi}_-^{k-1}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)},\end{aligned} \tag{6.12}$$

where $\tilde{\Xi}_{+}^{k+1} := A_{k+1}^{+}\Phi^{k+1}$, $\tilde{\Xi}_{-}^{k-1} := A_{k-1}^{-}\Phi^{k-1}$. Then it is easily seen that $\mathcal{G}(\Phi^{k+1}) = \mathcal{G}(\tilde{\Xi}_{+}^{k+1})$, $\mathcal{G}(\Phi^{k-1}) = \mathcal{G}(\tilde{\Xi}_{-}^{k-1})$. Therefore, using Lemma 11 and (6.12) we can see that there exists a constant $\breve{C}$ such that

$$\begin{aligned}\sum_{i=1}^{N}\|(\mathcal{G}(\Phi^{k+1}) - \mathcal{G}(\Phi^{k-1}))\varphi_i^k\|_{L^2(\mathbb{R}^3)}^2 &= \sum_{i=1}^{N}\|(\mathcal{G}(\tilde{\Xi}_{+}^{k+1}) - \mathcal{G}(\tilde{\Xi}_{-}^{k-1}))\varphi_i^k\|_{L^2(\mathbb{R}^3)}^2 \\ &\leq \breve{C}\|\tilde{\Xi}_{+}^{k+1} - \tilde{\Xi}_{-}^{k-1}\|_{\bigoplus_{i=1}^{N} L^2(\mathbb{R}^3)}^2 \\ &\leq \breve{C}\|D_{\Phi^{k+1}} - D_{\Phi^{k-1}}\|_2^2.\end{aligned}$$

Combining this inequality, (6.10) and (6.11) we obtain

$$|f(\Phi^k, \Phi^{k+1}, \mathbf{e}^k, \mathbf{e}^{k+1}) - \mu|^{1-\tilde{\theta}} \leq \tilde{\kappa}\breve{C}^{1/2}\|D_{\Phi^{k+1}} - D_{\Phi^{k-1}}\|_2, \tag{6.13}$$

for $k \geq k_1$.

Step 3. It follows from (6.5)–(6.7) and (6.13) that

$$\begin{aligned}&(\mathcal{E}(\Phi^k, \Phi^{k+1}) - \mu)^{\tilde{\theta}} - (\mathcal{E}(\Phi^{k+1}, \Phi^{k+2}) - \mu)^{\tilde{\theta}} \\ &\quad \geq \frac{\tilde{\theta}}{\tilde{\kappa}\breve{C}^{1/2}\|D_{\Phi^{k+1}} - D_{\Phi^{k-1}}\|_2}(2^{-1}\gamma\|D_{\Phi^{k+2}} - D_{\Phi^k}\|_2^2),\end{aligned}$$

for $k \geq k_1$. Since the sum of the left-hand side for $k = 1, 2, \dots$ is finite, the corresponding sum of the right-hand side is also convergent. Setting $\alpha_k := \|D_{\Phi^{k+1}} - D_{\Phi^{k-1}}\|_2$ this sum is written as

$$\frac{\tilde{\theta}\gamma}{2\tilde{\kappa}\breve{C}^{1/2}}\sum_{k=1}^{\infty}\frac{\alpha_{k+1}^2}{\alpha_k}.$$

Hence by Lemma 19 we can see that

$$\sum_{k=1}^{\infty}\alpha_k = \sum_{k=1}^{\infty}\|D_{\Phi^{k+1}} - D_{\Phi^{k-1}}\|_2,$$

is convergent.

Let us define unitary matrices $\tilde{A}_k$ so that

$$\|\tilde{A}_{k+1}\tilde{\Xi}_{-}^{k+1} - \tilde{A}_{k-1}\tilde{\Xi}_{-}^{k-1}\|_{\bigoplus_{i=1}^{N} L^2(\mathbb{R}^3)} = \|\tilde{\Xi}_{+}^{k+1} - \tilde{\Xi}_{-}^{k-1}\|_{\bigoplus_{i=1}^{N} L^2(\mathbb{R}^3)},$$

will hold for any $k \geq 1$. We set $\tilde{A}_0 := I, \tilde{A}_1 := I$, where I is the identity matrix. Assume that $\tilde{A}_{k-1}$ has been defined. Since $\tilde{A}_{k-1}$ is unitary and $\Xi_+^{k+1} = A_{k+1}^+(A_{k+1}^-)^{-1}\Xi_-^{k+1}$, we have

$$\begin{aligned}
&\|\tilde{\Xi}_+^{k+1} - \tilde{\Xi}_-^{k-1}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)} \\
&\quad = \|\tilde{A}_{k-1}A_{k+1}^+(A_{k+1}^-)^{-1}\tilde{\Xi}_-^{k+1} - \tilde{A}_{k-1}\tilde{\Xi}_-^{k-1}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)}.
\end{aligned}$$

Thus we should set $\tilde{A}_{k+1} := \tilde{A}_{k-1}A_{k+1}^+(A_{k+1}^-)^{-1}$. Consequently, we obtain

$$\begin{aligned}
\tilde{A}_{2k} &= A_2^+(A_2^-)^{-1}\cdots A_{2(k-1)}^+(A_{2(k-1)}^-)^{-1}A_{2k}^+(A_{2k}^-)^{-1}, \\
\tilde{A}_{2k+1} &= A_3^+(A_3^-)^{-1}\cdots A_{2(k-1)+1}^+(A_{2(k-1)+1}^-)^{-1}A_{2k+1}^+(A_{2k+1}^-)^{-1},
\end{aligned}$$

for $k \geq 1$. Now set $A_0 := I$, $A_1 := I$ and $A_{2k} := \tilde{A}_{2k}A_{2k}^-$, $A_{2k+1} := \tilde{A}_{2k+1}A_{2k+1}^-$ for $k \geq 1$. Then if we define $\Xi^k := A_k\Phi^k$ for $k \geq 0$, we have

$$\|\Xi^{k+1} - \Xi^{k-1}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)} = \|\tilde{\Xi}_+^{k+1} - \tilde{\Xi}_-^{k-1}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)}, \tag{6.14}$$

for any $k \geq 1$. Since $\{\Phi^k\}$ satisfies $\mathcal{F}(\Phi^k)\varphi_i^{k+1} = \epsilon_i^{k+1}\varphi_i^{k+1}$, $1 \leq i \leq N$, we can see that Ξ^k satisfies $\mathcal{F}(\Xi^k)\xi_i^{k+1} = \sum_{j=1}^N \epsilon_{ij}^{k+1}\xi_j^{k+1}$, $1 \leq i \leq N$, where ϵ_{ij}^k is the (i,j)th entry of the matrix $A_k(\mathrm{diag}\,[\epsilon_1^k, \ldots, \epsilon_N^k])A_k^{-1}$. Noting that A_k is a unitary matrix we have $\sum_{i,j=1}^N |\epsilon_{ij}^k|^2 = \sum_{i=1}^N |\epsilon_i^k|^2 \leq N|\inf\sigma(h)|^2$. Thus we can apply Lemma 20 to $\{\Xi^k\}$, which combined with (6.14) and (6.12) yields

$$\begin{aligned}
&\sum_{k=1}^{\infty}\|\Xi^{k+1} - \Xi^{k-1}\|_{\bigoplus_{i=1}^N H^2(\mathbb{R}^3)} \\
&\quad \leq 2\beta_\zeta\sum_{k=1}^{\infty}\|\Xi^{k+1} - \Xi^{k-1}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)} + \|\Xi^2 - \Xi^0\|_{\bigoplus_{i=1}^N H^2(\mathbb{R}^3)} \\
&\quad = 2\beta_\zeta\sum_{k=1}^{\infty}\|\tilde{\Xi}_+^{k+1} - \tilde{\Xi}_-^{k-1}\|_{\bigoplus_{i=1}^N L^2(\mathbb{R}^3)} + \|\Xi^2 - \Xi^0\|_{\bigoplus_{i=1}^N H^2(\mathbb{R}^3)} \\
&\quad \leq 2\beta_\zeta\sum_{k=1}^{\infty}\alpha_k + \|\Xi^2 - \Xi^0\|_{\bigoplus_{i=1}^N H^2(\mathbb{R}^3)} < \infty,
\end{aligned}$$

with $\zeta := N^{1/2}|\inf\sigma(h)|$. Thus there exist limits $\Xi^\infty := \lim_{k\to\infty}\Xi^{2k}$ and $\tilde{\Xi}^\infty := \lim_{k\to\infty}\Xi^{2k+1}$ in $\bigoplus_{i=1}^N H^2(\mathbb{R}^3)$. Now noting that $D_{\Xi^k} = D_{\Phi^k}$, that

$\lim_{k\to\infty} D_{\Xi^{2k}} = D_{\Xi^\infty}$, $\lim_{k\to\infty} D_{\Xi^{2k+1}} = D_{\tilde{\Xi}^\infty}$ with respect to the topology of $\mathcal{L}(L^2(\mathbb{R}^3))$, that $D_{\Phi^{2k}}$ and $D_{\Phi^{2k+1}}$ converge in $\mathcal{T}_2$, and that $\|\cdot\|_{\mathcal{L}(L^2(\mathbb{R}^3))} \leq \|\cdot\|_2$ (cf. [17, Theorem VI.22 (d)]) the results in Theorem 1 follow, and the proof is completed. □

Proof of Theorem 3. (1) Since Ξ^{2k} converges to Ξ^∞ in $\bigoplus_{i=1}^N H^2(\mathbb{R}^3)$, the operator $\mathcal{F}(\Phi^{2k}) - \mathcal{F}(\Xi^\infty) = \mathcal{G}(\Xi^{2k}) - \mathcal{G}(\Xi^\infty)$ converges to 0 in $\mathcal{L}(L^2(\mathbb{R}^3))$. Thus by the upper semicontinuity of the spectrum (see e.g. [10, Theorems IV 1.16 and IV 3.18]) and the uniform well-posedness, for any $\delta > 0$ there exist $k' \in \mathbb{N}$ and a constant $v \in \mathbb{R}$ such that the N smallest eigenvalues of $\mathcal{F}(\Xi^\infty)$ and $\mathcal{F}(\Phi^{2k})$ for $k \geq k'$ are smaller than v and the rest of the spectra of them are larger than $v + \gamma - \delta$, which proves (1) for $\mathcal{F}(\Xi^\infty)$. The proof for $\mathcal{F}(\tilde{\Xi}^\infty)$ is exactly the same.
(2) By the proof of (1) there exists a closed curve g in $\mathbb{C}$ such that the N smallest eigenvalues of $\mathcal{F}(\Xi^\infty)$ and $\mathcal{F}(\Phi^{2k})$ for $k \geq k'$ are enclosed by g, and the distances between g and the spectra of $\mathcal{F}(\Xi^\infty)$ and $\mathcal{F}(\Phi^{2k})$ for $k \geq k'$ are larger than $\gamma/3$. Thus using the representation $P_\Phi = -(2\pi i)^{-1} \oint_g (\mathcal{F}(\Phi) - z)^{-1} dz$ of the projections P_Φ to the direct sum of the eigenspaces of $\mathcal{F}(\Phi)$ we can see that $\lim_{k\to\infty} P_{\Phi^{2k}} = P_{\Xi^\infty}$ in $\mathcal{L}(L^2(\mathbb{R}^3))$. Hence with ξ_i^{2k+1} in the proof of Theorem 1 we have

$$\tilde{\xi}_i^\infty = \lim_{k\to\infty} \xi_i^{2k+1} = \lim_{k\to\infty} P_{\Phi^{2k}} \xi_i^{2k+1} = P_{\Xi^\infty} \tilde{\xi}_i^\infty,\ 1 \leq i \leq N,$$

where $\tilde{\Xi}^\infty = {}^t(\tilde{\xi}_1^\infty, \ldots, \tilde{\xi}_N^\infty)$. This means that $\tilde{\Xi}^\infty$ is an orthonormal basis of $\mathcal{H}_{\Xi^\infty} := \operatorname{Ran} P_{\Xi^\infty}$. In the same way we can also prove that Ξ^∞ is an orthonormal basis of the direct sum $\mathcal{H}_{\tilde{\Xi}^\infty} := \operatorname{Ran} P_{\tilde{\Xi}^\infty}$.

Let $\hat{\Phi}^\infty = {}^t(\hat{\varphi}_1, \ldots, \hat{\varphi}_N)$ be a tuple of the eigenfunctions of $\mathcal{F}(\Xi^\infty)$ corresponding to the N smallest eigenvalues $\hat{\epsilon}_1^\infty, \ldots, \hat{\epsilon}_N^\infty \in \mathbb{R}$ as above Theorem 3. Then $\hat{\Phi}^\infty$ is an orthonormal basis of $\mathcal{H}_{\Xi^\infty}$ and

$$\mathcal{F}(\Xi^\infty)\hat{\varphi}_i^\infty = \hat{\epsilon}_i^\infty \hat{\varphi}_i^\infty,\ 1 \leq i \leq N. \tag{6.15}$$

Thus $\hat{\Phi}^\infty$ and $\tilde{\Xi}^\infty$ are orthonormal bases of the same space $\mathcal{H}_{\Xi^\infty}$. Therefore, there exists a unitary matrix A_∞ such that $\tilde{\Xi}^\infty = A_\infty \hat{\Phi}^\infty$. We note here that $\mathcal{F}(\tilde{\Xi}^\infty) = \mathcal{F}(\hat{\Phi}^\infty)$ also holds.

Next we shall prove $\hat{\epsilon}_i^\infty = \lim_{k\to\infty} \epsilon_i^{2k+1}$, $1 \leq i \leq N$. From the proof of

Theorem 1 it follows that there exists a Hermitian matrix $(\tilde{\epsilon}_{ij}^{\infty})$ such that

$$\mathcal{F}(\Xi^{\infty})\tilde{\xi}_i^{\infty} = \sum_{j=1}^{N} \tilde{\epsilon}_{ij}^{\infty}\tilde{\xi}_j^{\infty},\ 1 \leq i \leq N.$$

Thus by (6.15) we can see that $\operatorname{diag}[\hat{\epsilon}_1^{\infty}, \dots, \hat{\epsilon}_N^{\infty}] = A_{\infty}^{-1}(\tilde{\epsilon}_{ij}^{\infty})A_{\infty}$. Since $(\tilde{\epsilon}_{ij}^{\infty})$ is the limit of the Hermitian matrices (ϵ_{ij}^{2k+1}) whose eigenvalues are $(\epsilon_1^{2k+1}, \dots, \epsilon_N^{2k+1})$, the perturbation theorem for the eigenvalues of Hermitian matrices (see e.g. [4, Problem 1.17]) yields $\hat{\epsilon}_i^{\infty} = \lim_{k\to\infty} \epsilon_i^{2k+1}$, $1 \leq i \leq N$.
(3) If $\Xi^{\infty} = \Theta\tilde{\Xi}^{\infty}$, we have $\mathcal{F}(\Xi^{\infty}) = \mathcal{F}(\tilde{\Xi}^{\infty})$ and thus

$$\mathcal{F}(\Xi^{\infty}) = \mathcal{F}(\tilde{\Xi}^{\infty}) = \mathcal{F}(\hat{\Phi}^{\infty}).$$

Hence by (6.15) we have

$$\mathcal{F}(\hat{\Phi}^{\infty})\hat{\varphi}_i^{\infty} = \hat{\epsilon}_i^{\infty}\hat{\varphi}_i^{\infty},\ 1 \leq i \leq N,$$

which means that $\hat{\Phi}^{\infty}$ is a solution to the Hartree-Fock equation.
(4) Assume that $\hat{\Phi}^{\infty}$ forms an orthonormal basis of the direct sum of the eigenspaces of the N smallest eigenvalues of $\mathcal{F}(\hat{\Phi}^{\infty})$. Then recalling that $\mathcal{F}(\hat{\Phi}^{\infty}) = \mathcal{F}(\tilde{\Xi}^{\infty})$ it follows that $\hat{\Phi}^{\infty}$ is an orthonormal basis of $\mathcal{H}_{\tilde{\Xi}^{\infty}}$. Since $\hat{\Phi}^{\infty}$ is an orthonormal basis also of $\mathcal{H}_{\Xi^{\infty}}$, we have $\mathcal{H}_{\tilde{\Xi}^{\infty}} = \mathcal{H}_{\Xi^{\infty}}$, which implies that Ξ^{∞} and $\tilde{\Xi}^{\infty}$ are orthonormal bases of the same space. Therefore, there exists a unitary matrix Θ such that $\Xi^{\infty} = \Theta\tilde{\Xi}^{\infty}$.
(5) This result follows from (2) if we prove that the necessary and sufficient condition that $\Phi, \tilde{\Phi} \in \mathcal{W}$ satisfy $D_{\Phi} = D_{\tilde{\Phi}}$ is that there exists a unitary matrix $\hat{A}$ such that $\Phi = \hat{A}\tilde{\Phi}$. The sufficiency is obvious. The necessity follows from that Φ is an orthonormal basis of $\operatorname{Ran} D_{\Phi}$, which was also mentioned in Section 1.□

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