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On the Hartree-Fock Time-dependent Problem

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Abstract. A previous result is generalized. An existence and uniqueness theorem is proved for the Hartree-Fock time-dependent problem in the case of a finite Fermi system interacting via a two body potential, which is supposed dominated by the kinetic energy part of the one-particle hamiltonian.

1. Introduction

In this paper we consider the existence problem for the Hartree-Fock time-dependent equations of a finite system of fermions. This problem was first solved using fixed point theorems for local contractions in Banach spaces in Ref. [1], for the case of a bounded two body potential, and in Ref. [2][1] for the case of the repulsive Coulomb potential.

In the present paper we extend those results to a general potential, bounded from below and "essentially" dominated by the one-particle hamiltonian (for instance the laplacian operator). Our main result is Proposition 5.5., which proves the existence and uniqueness of a global solution, both in the case of the classical and of the mild solution, according to the smoothness of the initial data[2].

2. Notations and Hypotheses

We denote by:

E a Hilbert space with inner product $\langle\cdot,\cdot\rangle$;

[1] The paper [1] considers the case of arbitrary N and not only the case $N=2$ like erroneously stated in Ref. [2].

[2] While this work was in preparation, we received a preprint by Chadam and Glassey [3], where formal proofs have been obtained for the case of the Coulomb potential. Furthermore Definition 2.1. of [3] must be revised since the expression $\|K\|_{1,1}=\mathrm{Tr}(A|K|A)$ does not satisfy the triangle inequality.

$\mathscr{L}(E)$ the set of all bounded linear operators in E, equipped with the norm topology $\|\cdot\|$;

$\mathscr{L}_1(E) \subset \mathscr{L}(E)$ the set of trace-class operators, equipped with the usual norm $\|\cdot\|_1 = \mathrm{Tr}|\cdot|$;

$$H(E) = \{T;\ T \in \mathscr{L}(E),\ T = T^*\}$$

$$H_1(E) = \{T;\ T \in \mathscr{L}_1(E),\ T = T^*\}.$$

Let $A : \mathscr{D}(A)\,(\subset E) \to E$ be a self-adjoint operator such that

$$A \geqq kI \quad \text{for a fixed} \quad k \in R.$$

Let

$$M = (A - k + 1)^{\frac{1}{2}}$$

and $\forall T \in \mathscr{L}_1(E)$, $\varphi_T : \mathscr{D}(M) \times \mathscr{D}(M) \to C$ be defined by

$$\varphi_T(x, y) = \langle TMx, My \rangle, \qquad x, y \in \mathscr{D}(M).$$

Let γ be the linear mapping defined by

$$\begin{cases} \mathscr{D}(\gamma) = \{T;\ T \in \mathscr{L}_1(E),\ \varphi_T \text{ is continuous in } E \times E\} \\ \langle \gamma(T)x, y \rangle = \bar{\varphi}_T(x, y) \end{cases}$$

where $\bar{\varphi}_T$ denotes the (unique) extension of φ_T to $E \times E$.

It is easy to show that $T \in \mathscr{D}(\gamma)$, $x \in \mathscr{D}(M) \Rightarrow \gamma(T)x = MTMx$ (see Ref. [4]).

We denote by

$$\mathscr{L}_1^A(E) = \{T;\ T \in \mathscr{L}_1(E) \text{ such that } MTM \in \mathscr{L}_1(E)\}$$

$$H_1^A(E) = \{T;\ T \in H_1(E) \text{ such that } MTM \in H_1(E)\}$$

we introduce a norm in $H_1^A(E)$ by putting

$$\|T\|_{1,A} = \mathrm{Tr}(|MTM|).$$

It is easy to see that this is indeed a norm which makes $H_1^A(E)$ a Banach space; moreover the following inequality holds

$$\|T\|_{1,A} \geqq \|M^{-1}\|^{-2}\, \|T\|_1.$$

Let $B : H_1^A(E) \to H(E)$ be a continuous linear map such that

i) $B(T)M^{-1}x \in \mathscr{D}(M)$, $\forall x \in E$;

ii) $C(\cdot) \in \mathscr{L}(H_1^A(E), H(E))$, where

$$C(T) = MB(T)M^{-1}, \qquad T \in H_1^A(E);$$

iii) $\forall T, S \in H_1^A(E)$ the following equality holds:

$$\mathrm{Tr}(B(T)S) = \mathrm{Tr}(B(S)T);$$

iv) $\exists k_1 \in R$ such that $B(T)T \geqq k_1$, $\forall T \in H_1^A(E)$, $0 \leqq T \leqq I$.

Moreover we put

$$f(T) = [B(T), T]_-$$

(where $[A, B]_- = AB - BA$).

We consider the following abstract Hartree-Fock problem: find a function $T(\cdot)\in C(R^+; H_1^A(E))$ such that

$$\begin{cases} i\,dT/dt=[A, T]_- +[B(T), T]_- \\ T(0)=T_0\,. \end{cases} \tag{2.1}$$

We give now some general definitions.

Definition 2.1. Let X be a Banach space, $f\in C(X)$ a continuous function on X and $-A$ the infinitesimal generator of a strongly continuous semigroup $G(t)$ such that $\|G(t)\|\leqq e^{\omega t}$, $\forall t\in R^+$, $\omega\in R$. A function $u:[0, T[\to X$ continuous on $[0, T[$ is called a mild solution of the problem

$$\begin{cases} u'+Au+f(u)=v, \quad u'=du/dt, \quad v\in C([0, T[, X) \\ u(0)=u_0, \quad u_0\in X \end{cases} \tag{2.2}$$

if the following equality holds:

$$u(t)=G(t)u_0-\int_0^t G(t-s)\,(f(u(s))-v(s))\,ds\,. \tag{2.3}$$

Definition 2.2. $u:[0, T]\to X$ is called a classical solution of problem (2.2) if $u\in C^1([0, T]; X)\cap C([0, T]; \mathscr{D}(A))$ and (2.2) is satisfied. $C^1([0, T]; X)$ is the set of continuously differentiable functions $[0, T]\to X$ and $C([0, T]; \mathscr{D}(A))$ is the B-space of the continuous functions $[0, T]\to\mathscr{D}(A)$, $\mathscr{D}(A)$ being endowed with the graph-norm.

3. General Results

The following lemma is well-known:

Lemma 3.1. *u is a mild solution of problem* (2.2) *if and only if*

$$\exists (u_n)_{n\in N} \quad in \quad C^1([0, T]; X)\cap C([0, T]; \mathscr{D}(A))$$

such that

$$\begin{cases} u_n \xrightarrow[n\to\infty]{} u \\ u_n'+Au_n+f(u_n) \xrightarrow[n\to\infty]{} v \end{cases} \quad in \quad C([0, T]; X) \tag{3.1}$$

We say also that u is a mild solution of problem (2.2) *if and only if u is a strong solution in the sense of Friedrichs.*

Proposition 3.2 (Segal [5]). *Suppose f is locally Lipschitz. Then there exists $\tau\in R^+$ such that in $[0, \tau[$ there exists a unique mild solution of problem* (2.2). *Moreover if $u_0\in\mathscr{D}(A)$ then this solution is a classical solution.*

We put

$$T_0=\sup\{T>0;\ T \text{ such that in } [0, T] \text{ there exists a mild solution of problem (2.2)}\}\,.$$

Proposition 3.2. then implies that a unique mild solution u for the problem (2.2) is defined in $[0, T_0[$; we call such solution a *maximal solution* of problem (2.2).

For completeness we will prove the following

Proposition 3.3. *Let* $u:[0, T_0[\to X$ *be the maximal (mild) solution of problem* (2.2). *Let us suppose that*

i) $\exists M>0$ *such that* $\|u(t)\|\leqq M$, $\forall t\in[0, T_0[$;

ii) $B\subset X$ *is a bounded set* $\Rightarrow f(B)$ *is bounded in* X; *then* $T_0=+\infty$.
then $T_0=+\infty$.

Proof. It is enough to prove that $\exists \lim_{t\to T_0-} u(t)$. Indeed we shall prove that

$$\lim_{t\to T_0-} u(t)=G(T_0)u_0-\int_0^{T_0} G(T_0-s)(f(u(s))-v(s))\,ds\,.$$

We note that the integral on the R.H.S. must be understood in the Bochner's sense; obviously it exists because of hypothesis ii) and of the continuity of the functions involved.

Then we obtain

$$\begin{aligned}&\|u(t)-G(T_0)u_0+\int_0^{T_0} G(T_0-s)(f(u(s))-v(s))\,ds\|\\&\leqq\|G(t)u_0-G(T_0)u_0\|+\int_t^{T_0} e^{\omega(T_0-s)}\|f(u(s))-v(s)\|\,ds\\&\quad+\int_0^t\|G(T_0-s)(f(u(s))-v(s))-G(t-s)(f(u(s))-v(s))\|\,ds\,.\end{aligned}$$

The first two terms are easily seen to converge to zero because of the strong continuity property of $G(\cdot)$ and of hypotheses i) and ii). The third term converges to zero because of the dominated convergence theorem. This completes the proof of the Proposition.

4. Preliminary Results

Definition 4.1. $\forall T\in H_1^A(E)$ let $\psi_T:\mathscr{D}(AM)\times\mathscr{D}(AM)\to C$ be defined by[3]

$$\psi_T(x,y)=-i\langle TMx, AMy\rangle+i\langle TAMx, My\rangle\,. \tag{4.1}$$

If ψ_T is continuous we denote by ψ_T its unique extension to $E\times E$.

Definition 4.2. Let $a:H_1^A(E)\to H_1^A(E)$ be defined by

$$\begin{cases}\mathscr{D}(a)=\{T;\ T\in H_1^A(E),\ \psi_T \text{ is continuous on } E\times E\}\\ \langle a(T)x,y\rangle=-i<Tx,Ay\rangle+i\langle Ax,Ty\rangle, \quad x,y\in E\,.\end{cases} \tag{4.2}$$

It is easy to see that $T\in\mathscr{D}(a)$, $x\in\mathscr{D}(A)\Rightarrow Tx\in\mathscr{D}(A)$ and $a(T)x=[A,T]_-x$.

Proposition 4.3. $\forall t\in R^+\cup\{0\}$ *we put*

$$G_t(T)=e^{-itA}Te^{itA},\qquad T\in H_1^A(E)\,; \tag{4.3}$$

then $t\mapsto G_t(\cdot)$ *is a strongly continuous contraction semigroup on* $H_1^A(E)$. *Moreover its infinitesimal generator is the linear map* a *of Definition 4.2.*

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[3] We suppose $\mathscr{D}(AM)$ to be dense in E.

Proof. We have

$$MG_t(T)M = G_t(MTM) \qquad \forall T \in H_1^A(E), \tag{4.4}$$

so that

$$\mathrm{Tr}(MG_t(T)M) = \mathrm{Tr}(MTM). \tag{4.5}$$

It follows that

$$\mathrm{Tr}(|MG_t(T)M|) = \|e^{-itA}MTMe^{itA}\|_1 \leqq \mathrm{Tr}(|MTM|) = \|T\|_{1,A}$$

which proves that $G_t(\cdot)$ operates on $H_1^A(E)$ and it is a contraction semigroup. Now

$$MG_t(T)M - MTM = G_t(MTM) - MTM$$

so that

$$\|G_t(T) - T\|_{1,A} = \|G_t(MTM) - MTM\|_1$$

and the strong continuity follows from Proposition 3.4. of [1]. The last part of the proposition follows from the analogue of Lemma 3.3. of [1] and from [4].

Proposition 4.4. *Let* $T \in \mathscr{D}(a)$, *then* $\mathrm{Tr}(M[A, T]_- M) = 0$.

Proof. If $T \in \mathscr{D}(a)$ the Hille-Yosida theorem implies that

$$a(T) = \lim_{h \to 0+} h^{-1}(G_h(T) - T)$$

where the limit is understood in the $H_1^A(E)$-norm. Then we have

$$\mathrm{Tr}(Ma(T)M) = \lim_{h \to 0+} h^{-1}(\mathrm{Tr}(MG_h(T)M) - \mathrm{Tr}(MTM)) = 0$$

which completes the proof.

For what concerns the non-linear part we have the following

Proposition 4.5. $f \in C^1(H_1^A(E))$ *(i.e. f is continuously Fréchet differentiable in $H_1^A(E)$) and the following equality holds:*

$$f'(T)(S) = [B(S), T]_- + [B(T), S]_-, \qquad T, S \in H_1^A(E).$$

Proof. $T \in H_1^A(E) \Rightarrow f(T) \in H_1^A(E)$. Indeed we have

$$\begin{aligned}\mathrm{Tr}(|Mf(T)M|) &\leqq \mathrm{Tr}(|MB(T)TM|) + \mathrm{Tr}(|MTB(T)M|)\\ &= \|MB(T)TM\|_1 + \|MTB(T)M\|_1 = 2\|MB(T)M^{-1}MTM\|_1\\ &\leqq 2\|MB(T)M^{-1}\| \, \|T\|_{1,A} = 2\|C(T)\| \, \|T\|_{1,A}\\ &\leqq 2C_1 \|T\|_{1,A}^2.\end{aligned}$$

where C_1 denotes some positive constant. For the differentiability of f we have:

$$f(T+S) - f(T) = [B(T), S]_- + [B(S), T]_- + [B(S), S]_-$$

and

$$[B(S), S]_- / \|S\|_{1,A} \xrightarrow[S \xrightarrow{H_1^A(E)} 0]{H_1^A(E)} 0$$

by an argument similar to that given above.

5. A priori Inequalities and Existence Theorems

The results of the preceding section and Proposition 3.2. imply the following

Proposition 5.1. *There exists a unique local mild solution for the problem* (2.1). *Moreover if* $T_0 \in \mathscr{D}(a)$ *then the solution is a classical solution.*

Lemma 5.2. *Let* $M_n = nM(n+M)^{-1}$, $n \in N$, *be the n-th Yosida approximant for M, so that, as is well-known,* $\|M_n x\| \leqq \|Mx\|$, $\lim_{n\to\infty} M_n x = Mx$, $\forall x \in \mathscr{D}(M)$. *Then if* $T \in H_1^A(E)$ *we have*

$$\operatorname{Tr}(MTM) = \lim_{n\to\infty} \operatorname{Tr}(M_n T M_n). \tag{5.1}$$

Proof. Without loss of generality we can suppose $T \geqq 0$. Otherwise, noting that $T = T^+ - T^-$, T^+, $T^- \geqq 0$, we can reason separately on each of them. Let[4]

$$Tx = \sum_{k=1}^{\infty} \lambda_k \langle x, e_k \rangle e_k, \quad \lambda_k \in R^+ \cup \{0\} \forall k \in N.$$

Then

$$\operatorname{Tr}(MTM) = \sum_{k=1}^{\infty} \lambda_k \|Me_k\|^2$$

$$\operatorname{Tr}(M_n T M_n) = \sum_{k=1}^{\infty} \lambda_k \|M_n e_k\|^2.$$

Now $\forall \varepsilon \in R^+$ we can choose $m_\varepsilon \in N$ such that

$$\sum_{k=m_\varepsilon+1}^{\infty} \lambda_k \|Me_k\|^2 < \varepsilon/3$$

so that

$$\begin{aligned}|\operatorname{Tr}(MTM) - \operatorname{Tr}(M_n T M_n)| &\leqq \sum_{k=1}^{m_\varepsilon} \lambda_k \big| \|Me_k\|^2 - \|M_n e_k\|^2 \big| \\ &\quad + 2 \sum_{k=m_\varepsilon+1}^{\infty} \lambda_k \|Me_k\|^2 < \varepsilon/3 + 2\varepsilon/3 = \varepsilon\end{aligned}$$

if $n > n_\varepsilon$, where $n_\varepsilon \in N$ is suitably chosen. This completes the proof of the lemma.

Proposition 5.3. *Let T be a local solution of problem* (2.1) *with* $T_0 \in \mathscr{D}(a)$, *so that T is a classical solution. Then*

$$\operatorname{Tr}(MTM) + \tfrac{1}{2}\operatorname{Tr}(TB(T)) = \operatorname{Tr}(MT_0M) + \tfrac{1}{2}\operatorname{Tr}(T_0 B(T_0)) \tag{5.2}$$

Proof. We have

$$\begin{aligned}(id/dT)\operatorname{Tr}(MT(t)M) &= \operatorname{Tr}(M[A, T]_- M) + \operatorname{Tr}(M[B(T), T]_- M) \\ &= \operatorname{Tr}(M[B(T), T]_- M)\end{aligned}$$

by Proposition 4.4.

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[4] We suppose $\{e_k; k \in N\}$ to be a complete orthonornal system in E.

Because of hypothesis iii) on B we obtain

$$\tfrac{1}{2}(id/dT)\,\mathrm{Tr}(B(T)T) = i\,\mathrm{Tr}(B(T(t))\,\dot{T}(t))$$
$$= \mathrm{Tr}(B(T)[A, T]_-) + \mathrm{Tr}(B(T)[B(T), T]_-)$$
$$= \mathrm{Tr}(B(T)[A, T]_-)\,.$$

Recalling the definition of M, by Lemma 5.2. we can conclude

$$id/dt(\mathrm{Tr}(MTM) + \tfrac{1}{2}\mathrm{Tr}(TB(T))) = \mathrm{Tr}(M[B(T), T]_- M) + \mathrm{Tr}(B(T)[A, T]_-) = 0$$

so that the desired conclusion easily follows.

Proposition 5.4. *Let* $T_0 \in H_1^A(E)$ *and* T *be the mild solution of the problem* (2.1), *then* (5.2) *still holds.*

Proof. By Lemma 3.1 there exists $(T_n)_{n\in N}$ such that T_n is a classical solution of problem (2.1), i.e.

$$\begin{cases} T_n \xrightarrow[n\to\infty]{H_1^A(E)} T \\ iT_n' - [A, T_n]_- - [B(T_n), T_n]_- = S_n \xrightarrow[n\to\infty]{H_1^A(E)} 0\,. \end{cases}$$

Then we have, as in Proposition 5.3.,

$$(id/dT)\,[\mathrm{Tr}(MT_nM + \tfrac{1}{2}T_nB(T_n))] = \mathrm{Tr}(MS_nM) + \mathrm{Tr}(B(T_n)S_n) \xrightarrow[n\to\infty]{} 0$$

and this proves the assertion.

Proposition 5.5. *If* $0 \leqq T_0 \leqq I$ *then* T *can be extended to all the positive real axis. Moreover if* $T_0 \in \mathscr{D}(a)$ *then* T *is the unique global classical solution.*

Proof. It is enough to verify hypothesis i) of Proposition 3.3. From (5.2) it is easily seen that

$$\mathrm{Tr}(MT(t)M) \leqq C', \qquad C' \in R^+\,.$$

Now $0 \leqq T_0 \leqq I$ implies (see [1], Proposition 4.3.) that

$$\mathrm{Tr}(|MTM|) = \mathrm{Tr}(MTM)$$

and this proves the assertion.

6. The Hartree-Fock Time-dependent Problem

Let

$$E = L^2(R^3)\,.$$

The operator A of problem (2.1) can be interpreted as the kinetic energy operator (i.e. $-\Delta$) in the case of nuclear or molecular physics and as the kinetic energy plus an attractive central Coulomb potential in the case of atomic physics.

The operator B is defined as follows:

$$B(T)\varphi = B_D(T)\varphi - B_{EX}(T)\varphi, \qquad \varphi \in L^2(R^3)\,,$$

(the so-called "direct" and "exchange" potentials) where, if $T(x, y)$ denotes the kernel of T, we have

$$(B_D(T)\varphi)(x) = \left(\int_{R^3} v(x-y)\,T(y,y)\,dy\right)\varphi(x)$$

$$(B_{EX}(T)\varphi)(x) = \int_{R^3} v(x-y)\,T(x,y)\,\varphi(y)\,dy\,.$$

Here $v: R^3 \to R$ is the two body interaction potential, which we suppose to be differentiable almost everywhere.

Then

$$M = \left(-\Delta + \frac{z}{\|x\|} + k\right)^{\frac{1}{2}} \quad \text{in the case of atomic physics}$$

$$M = (-\Delta + 1)^{\frac{1}{2}} \qquad \text{in the case of nuclear or molecular physics.}$$

It is easy to see that $\mathscr{D}(M) = H^1(R^3)$.

Let $\{\varphi_k; k \in N\}$ be an orthonormal complete system in $L^2(R^3)$ such that $\varphi_k \in \mathscr{D}(M)$. We write the one-particle density matrix in the form*

$$T(x, y) = \sum_{k=1}^{\infty} \lambda_k \varphi_k(x)\overline{\varphi_k(y)} \tag{6.1}$$

$$0 \leqq \lambda_k \leqq 1\,, \qquad \forall k \in N\,. \tag{6.2}$$

Since we consider only systems with finite total number of particles we have

$$\sum_{k=1}^{\infty} \lambda_k < +\infty\,.$$

$T \in H_1^A(E)$ implies that

$$\mathrm{Tr}(|MTM|) = \mathrm{Tr}(MTM) = \sum_{k=1}^{\infty} \lambda_k \|M\varphi_k\|_2^2 < +\infty\,. \tag{6.3}$$

If we denote by v the linear operator defined by

$$(v\varphi)(x) = v(x)\,\varphi(x)$$

we suppose that

$$\|v\varphi\|_2 \leqq C\|M\varphi\|_2\,, \qquad \forall \varphi \in \mathscr{D}(v) \cap \mathscr{D}(M)\,.$$

Now the conditions on the linear part A are easily verified. Let us show that B verifies conditions i), ..., iv).

iii) and iv) are trivial.

i) Let us consider B_D:

$$(B_D(T)M^{-1}\varphi)(x) = \alpha_T(x)\,(M^{-1}\varphi)(x)$$

where

$$\alpha_T(x) = \int v(x-y)\,T(y,y)\,dy\,.$$

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* *Note Added in Proof.* It is enough to consider $T \geqq 0$; indeed for any T we can write $T = T_1 - T_2$, $T_1 \geqq 0$, $T_2 \geqq 0$, $T_1 = M^{-1}(MTM)^+ M^{-1}$, $T_2 = M^{-1}(MTM)^- M^{-1}$, so that $\|T\|_{1,A} = \|T_1\|_{1,A} + \|T_2\|_{1,A}$ and $B(T)$ is continuous on $H_1^A(E)$. We thank Prof. Chadam for a comment on this point.

Now $\alpha_T \in L^\infty(R^3)$ and

$$\|\alpha_T\|_\infty \leqq \sum_{k=1}^{\infty} \lambda_k \| \int v(x-y)|\varphi_k(y)|^2\,dy\|_\infty$$

$$\leqq C \sum_{k=1}^{\infty} \lambda_k \|M\varphi_k\|_2^2 = C\,\mathrm{Tr}(MTM) = C\|T\|_{1,A}\ ^{5} \tag{6.4}$$

Moreover we have

$$\|D_i\alpha_T\|_\infty \leqq C \sum_{k=1}^{\infty} \lambda_k \| \int v(x-y) D_i|\varphi_k(y)|^2\,dy\|_\infty$$

$$\leqq C \sum_{k=1}^{\infty} \lambda_k \|M\varphi_k\|_2^2 = C\|T\|_{1,A}\,. \tag{6.5}$$

This proves that $B_D(T)M^{-1}\varphi \in \mathscr{D}(M) = H^1(R^3)$.

For what concerns B_{EX} it is enough to note that

$$|D_i \int v(x-y)\overline{\varphi_k(y)}\varphi(y)\,dy| \leqq C\|M\varphi_k\|_2\ \|M\varphi\|_2 \tag{6.6}$$

hence condition i) is completely verified by analogous calculations.

Let us now verify condition ii).

Let $\varphi \in C_0^\infty(R^3)$; we consider

$$\langle MB(T)M^{-1}\varphi, \varphi\rangle = \langle B(T)M^{-1}\varphi, M\varphi\rangle$$

we have

$$\|B(T)M^{-1}\varphi\|_{H^1(R^3)}^2 = \|B(T)M^{-1}\varphi\|_2^2 + \sum_{i=1}^{3} \|D_i(B(T)M^{-1}\varphi)\|_2^2$$

$$\leqq C\|T\|_{1,A}^2\ \|M^{-1}\varphi\|_{H^1(R^3)}^2$$

as it can be seen by relations (6.4), (6.5), (6.6); hence

$$|\langle MB(T)M^{-1}\varphi, \varphi\rangle| \leqq \|B(T)M^{-1}\varphi\|_{H^1(R^3)}\ \|M\varphi\|_{H^{-1}(R^3)}$$

$$\leqq C\|T\|_{1,A}\ \|M^{-1}\varphi\|_{H^1(R^3)}\ \|M\varphi\|_{H^{-1}(R^3)}$$

$$\leqq C\|T\|_{1,A}\ \|\varphi\|_2^2\,,$$

so that condition ii) is proved by use of a density argument.

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[5] Here and in the following C denotes a suitable positive constant.