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An Existence Proof for the Hartree-Fock Time-dependent Problem with Bounded Two-Body Interaction

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Abstract. Using fixed point theorems for local contractions in Banach spaces, an existence and uniqueness proof for the Hartree-Fock time-dependent problem is given in the case of a finite Fermi system interacting via a bounded two-body potential. The existence proof for the "strong" solution of the evolution problem is obtained under suitable conditions on the initial state.

1. Introduction

In general, starting from a quasi-free (or generalized-free) state ϱ of a finite or infinite Fermi system at the time $t=t_0$, the natural evolution of the system gives rise to a state ϱ_t which does not remain quasi-free for $t>t_0$, and trustworthy methods of successive approximations for solving the evolution problem except in trivial cases are not known. An approximate procedure for solving this problem is provided by the time-dependent Hartree-Fock theory, first obtained by Dirac [1] and afterwards generalized by Bogoliubov [2] and Valatin [3]. These equations can be obtained by considering the evolution of the one-particle density matrix T and assuming that ϱ_t remains quasi-free in a given time interval. Perturbative solutions of such equations for superconducting systems have been studied by Di Castro and Young [4].

In spite of the simplicity of the approach, the equation of motion for the one-particle density matrix T is non-linear so that the existence problem is not easy even in the most simple physical cases. Written in matrix form the equation in the gauge-invariant case is of the type (see e.g. Ref. [5]):

$$i\frac{dT}{dt}=[A+U,T]_- \tag{1.1}$$

where A is the kinetic energy operator and U is the self-consistent potential which is a linear function of T. U is the difference of two terms: $U=U_D-U_{EX}$, where U_D denotes the "local" part and U_{EX} the exchange part. Neglecting the spin coordinates, which are completely unessential for our purposes, and denoting by q the space coordinate, by φ a one-particle wave-function, by $v(q,q')$ the two-body potential, and by $T(q,q')$ the "matrix element" of T in the coordinate representation, we have:

$$(U_D\varphi)(q)=[\int v(q,q')\,T(q',q')\,d^3q']\,\varphi(q) \tag{1.2}$$

$$(U_{EX}\varphi)(q)=-\int v(q,q')\,T(q,q')\,\varphi(q')\,d^3q'\,. \tag{1.3}$$

Of course, Eq. (1.1) has to be solved with the given initial condition $T|_{t=0}=T_0$.

We give here an existence and uniqueness proof for the solution of Eq. (1.1), assuming that the total number of particles is finite ($N=\int T(q,q)\,d^3q<+\infty$) and the two-particle potential $v(q,q')$ is bounded: $\sup_{q,q'}|v(q,q')|<+\infty$.

2. Notations and Hypotheses

We denote by:

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

$\mathscr{L}(E)$ the set of all bounded linear operators defined 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 $\|\cdot\|_1=Tr|\cdot|$.

$\mathscr{L}(\mathscr{L}_1(E),\mathscr{L}(E))$ the Banach space of all linear continuous mappings $\mathscr{L}_1(E)\to\mathscr{L}(E)$, equipped with the usual norm $|||\cdot|||$ topology.

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

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

$$C(0,\tau;H_1(E))=\{f;f:[0,\tau]\to H_1(E),\ f\ \text{continuous}\}$$

where $\tau>0$; C is a real Banach space equipped with the norm $\|f\|=\sup\{\|f(t)\|_1,\ t\in[0,\tau]\}$.

Let $\tau\in\mathbb{R}_+$, $T_0\in H_1(E)$, $A:D_A(\subseteq E)\to E$ a self-adjoint operator, $B\in\mathscr{L}(\mathscr{L}_1(E),\mathscr{L}(E))$ such that:

$$T\in H_1(E)\to B(T)\in H(E). \tag{2.1}$$

We consider the following problem: find a function $T(\cdot) \in C(0, \tau; H_1(E))$ such that:

$$\begin{cases} i\dfrac{dT}{dt} = [A, T]_- + [B(T), T]_- \\ T(0) = T_0 . \end{cases} \tag{2.2}$$

Definition 2.1. A function $T \in C(0, \tau; H_1(E))$ is called a *mild* solution of the problem (2.2) if the following equality holds:

$$T(t)x = e^{-itA} T_0 e^{itA} x + i \int_0^t e^{-i(t-s)A} [T(s), B(T(s))]_- e^{i(t-s)A} x \, ds \tag{2.3}$$

for every $x \in E$.

Definition 2.2. A function $T \in C(0, \tau; H_1(E))$ is called a *classical* solution of problem (2.2) if the following conditions are satisfied:

i) $T(\cdot)$ is continuously differentiable on the interval $[0, \tau]$;

ii) $\forall x \in D_A$, $\forall t \in [0, \tau]$, we have $T(t)x \in D_A$ and

$$\begin{cases} i\dfrac{dT(t)}{dt} x = A\,T(t)x - T(t)Ax + [B(T(t)), T(t)]_- x \\ T(0)x = T_0 x . \end{cases} \tag{2.4}$$

It is easy to show that if A is a bounded operator defined on E the mild solution is also a classical solution.

3. Preliminary Results

Definition 3.1. For every $T \in H_1(E)$ we define a mapping $\varphi_T : D_A \times D_A \to \mathbb{C}$ by the following relation:

$$\varphi_T(x, y) = -i\langle Tx, Ay\rangle + i\langle Ax, Ty\rangle, \forall (x, y) \in D_A \times D_A . \tag{3.1}$$

If φ_T is continuous on $D_A \times D_A$ with respect to the product topology, we denote by the same symbol the unique extension to $E \times E$ of φ_T.

Definition 3.2. Let a be the linear mapping defined by

$$\begin{cases} D_a = \{T;\ T \in H_1(E),\ \varphi_T \text{ is continuous with respect to the product topology of } E \times E\} \\ \langle a(T)x, y\rangle = \varphi_T(x, y)\ \forall T \in D_a, \forall (x, y) \in E \times E . \end{cases} \tag{3.2}$$

It is easy to show that $T \in D_a$, $x \in D_A$ implies $Tx \in D_A$ and the following equality holds

$$a(T)x = -iATx + iTAx \tag{3.3}$$

(see Ref. [8]).

Lemma 3.3. *Let a have the same meaning as before; then the spectrum* $\sigma(a) \subset i\mathbb{R}$ *and*

$$(\lambda - a)^{-1}(T)x = \int_0^\infty e^{-\lambda t} e^{-itA} T e^{itA} x \, dt, \qquad \forall \lambda \in \mathbb{C}, \ \mathrm{Re}\lambda > 0, \ \forall x \in E, \ T \in H_1(E). \tag{3.4}$$

Proof. A detailed proof of relation (3.4) can be found in Ref. [8]. The statement $\sigma(a) \subset i\mathbb{R}$ then follows easily.

Proposition 3.4. *a is the infinitesimal generator of a contraction semigroup in* $H_1(E)$ *and the following relation holds:*

$$e^{ta}(T) = e^{-itA} T e^{itA}, \qquad \forall T \in H_1(E). \tag{3.5}$$

Proof. Since e^{itA} is unitary, we have

$$\|e^{-itA} T e^{itA}\|_1 = \|T\|_1. \tag{3.6}$$

The semigroup property can be checked in a trivial way, so that we have only to prove that:

$$\lim_{t \to 0^+} e^{-itA} T e^{itA} = T \qquad \forall T \in H_1(E). \tag{3.7}$$

Since the set of finite rank operators is dense in $\mathscr{L}_1(E)$ in the trace-norm topology $\|\cdot\|_1$, we can restrict ourselves to prove Eq. (3.7) for an arbitrary projection operator of rank one.

Let T be defined by

$$Tx = \langle x, y \rangle y \qquad \forall x \in E, \ \|y\| = 1.$$

We have:

$$(e^{-itA} T e^{itA} - T)x = \langle x, e^{-itA} y \rangle e^{-itA} y - \langle x, y \rangle y.$$

The two-dimensional subspace generated by y and $e^{-itA} y$ is invariant with respect to the operator $e^{-itA} T e^{itA} - T$; so the eigenvalue problem is easily solved and one finds for the non-vanishing eigenvalues of $e^{-itA} T e^{itA} - T$:

$$\lambda = \pm(1 - |\langle e^{-itA} y, y \rangle|^2)^{\frac{1}{2}}.$$

It follows that

$$\|e^{-itA} T e^{itA} - T\|_1 = 2\sqrt{1 - |\langle e^{-itA} y, y \rangle|^2} \xrightarrow[t \to 0^+]{} 0.$$

Hence the semigroup defined by (3.7) is strongly continuous. By Lemma 3.3 a is the infinitesimal generator of this semigroup.

Let

$$\gamma(T) = -i[B(T), T] \qquad \forall T \in H_1(E) \tag{3.8}$$

then $\gamma: H_1(E) \to H_1(E)$ is a continuous mapping and

$$\|\gamma(T)\|_1 \leqq 2|||B||| (\|T\|_1)^2 . \tag{3.9}$$

Proposition 3.5. *The following statements are true:*
i) γ *is locally lipschitzian on* $H_1(E)$.
ii) γ *is differentiable and*

$$\gamma'(T) \cdot S = -i[B(S), T] - i[B(T), S] .$$

iii) *The following inequality holds*

$$\|T\|_1 \leqq \|T - \alpha\gamma(T)\|_1, \quad \forall T \in H_1(E), \ \forall \alpha \in \mathbb{R}_+ . \tag{3.10}$$

Proof. i) Let $\|T\|_1, \|S\|_1 \leqq r, r > 0$; then

$$\begin{aligned} \|\gamma(T) - \gamma(S)\|_1 &= \|[B(T), T]_- - [B(T), S]_- + [B(T), S]_- - [B(S), S]_- \|_1 \\ &\leqq \|[B(T), T - S]_- \|_1 + \|[B(T - S), S]_- \|_1 \\ &\leqq 4|||B||| \, r \, \|T - S\|_1 ; \end{aligned}$$

ii) can be directly verified.
iii) Let $\alpha > 0$, $T \in H_1(E)$, and

$$T - \alpha\gamma(T) = S . \tag{3.11}$$

Denoting by $\{\lambda_i\}$ the set of the eigenvalues of T and by $\{u_i\}$ a corresponding set of orthonormal eigenvectors, we can write:

$$Tx = \sum_{i=1}^{\infty} \lambda_i \langle x, u_i \rangle u_i . \tag{3.12}$$

Defining:

$$\sigma(T)x = \sum_{i=1}^{\infty} \operatorname{sign}(\lambda_i) \langle x, u_i \rangle u_i \tag{3.13}$$

$$|T| x = \sum_{i=1}^{\infty} |\lambda_i| \langle x, u_i \rangle u_i \tag{3.14}$$

since

$$Tr[\gamma(T)\,\sigma(T)] = Tr[\sigma(T)\,\gamma(T)] = 0 \tag{3.15}$$

it follows that:

$$\begin{aligned} \|T\|_1 &= \tfrac{1}{2} Tr(S\sigma(T) + \sigma(T)S) \\ &\leqq \tfrac{1}{2} Tr(|S\sigma(T) + \sigma(T)S|) \leqq \|\sigma(T)\| \, \|S\|_1 = \|S\|_1 \end{aligned} \tag{3.16}$$

which proves (3.10).

4. The Existence Theorem

Let X be a real Banach space (with norm $\| \ \|_X$), $C(0,\tau;X)$ the Banach space of the continuous mappings $[0,\tau]\to X$ equipped with the norm $\|\cdot\| = \mathrm{Sup}\{\|\cdot(t)\|_X, t\in[0,\tau]\}$, M the infinitesimal generator of a contraction semigroup $t\to e^{tM}$ in X. $f:X\to X$ a locally lipschitzian mapping[1] such that:

$$\|x\|_X \leqq \|x-\alpha f(x)\|_X \quad \forall \alpha\geqq 0,\ x\in X. \tag{4.1}$$

We consider the following integral equation:

$$u(t)=e^{tM}u_0+\int_0^t e^{(t-s)M} f[u(s)]\,ds \tag{4.2}$$

where u_0 is a given element in X and $u\in C(0,\tau;X)$.

Then the following theorem holds: (for the proof see Refs. [6, 7, 11]).

Theorem 4.1. *There exists a unique solution of the problem* (4.2). *This solution depends continuously upon the initial condition. Furthermore, if $u_0\in D_M$ and is differentiable in X, then u is differentiable in $[0,\tau]$, $u(t)\in D_M$ $\forall t\in[0,\tau]$ and we have*

$$\begin{cases} \dfrac{du(t)}{dt} = M u(t) + f[u(t)] \\ u(0)=u_0 . \end{cases} \tag{4.3}$$

Applying Theorem 4.1 to our case, we obtain:

Theorem 4.2. *$\forall T_0\in H_1(E)$ there exists a unique mild solution $T(\cdot)$ of Eq.* (2.2). *Furthermore, if the mapping*

$$(x,y)\to\langle T_0x, Ay\rangle+\langle Ax, T_0y\rangle \qquad \forall(x,y)\in D_A\times D_A$$

is continuous with respect to the product topology of $E\times E$, then $T(\cdot)$ is a classical solution which depends continuously upon the initial condition.

Proof. It is enough to apply Theorem 4.1 with $f=\gamma$, $M=a$, $X=H_1(E)$ and use Propositions 3.4, 3.5.

Proposition 4.3. *If $T(\cdot)$ is a mild solution of problem* (2.2) *then for any $t\in[0,\tau]$ there exists a self-adjoint operator $K(t)$ such that*

$$T(t)=e^{-iK(t)}T_0e^{iK(t)}. \tag{4.4}$$

Proof. Let $T_0\in D_a$ and $T(\cdot)$ be the classical solution of problem (2.2). We put $Q(t)=B(T(t))$, $t\in[0,\tau]$; Q is a Lipschitz continuous mapping $[0,\tau]\to H(E)$. It is easy to see that for the linear problem

$$\begin{cases} i\dfrac{du}{dt}=\big(A+B(T(t))\big)u(t) \\ u(t_0)=u_0 \end{cases} \tag{4.5}$$

[1] By locally lipschitzian we mean that for any $r>0$, $u\in X$, $v\in X$, $\|u\|_X\leqq r$, $\|v\|_X\leqq r$, $\exists N_r>0$ such that $\|f(u)-f(v)\|_X\leqq N_r\|u-v\|_X$.

there exists a unitary Green function $U(t, s)$. It follows [8] that the problem

$$\begin{cases} i\dfrac{dS(t)}{dt} = [A + B(T(t)), S(t)]_- \\ S(0) = T_0 \end{cases} \tag{4.6}$$

has a unique classical solution given by

$$S(t) = U(t, 0)\, T_0\, U(-t, 0)\,. \tag{4.7}$$

Furthermore $T(\cdot)$ is obviously a solution of (4.6), so that, from the uniqueness of the solution, we have $S = T$.

For any $t \in [0, \tau]$ let $K(t)$ be the self-adjoint operator such that $U(-t, 0) = e^{iK(t)}$; Eq. (4.4) then follows.

If $T_0 \in H_1(E)$ we can prove (4.7) by a straightforward argument of density, since D_a is dense in $H_1(E)$.

5. The Hartree-Fock Time-dependent Problem

We now give sufficient conditions in order that Eq. (1.1) be solvable by the methods of Section 4.

Let $E = \mathscr{L}^2(R^3)$ be the one-particle Hilbert space. We assume that the two-particle potential $v(q, q')$

$$v : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R} \tag{5.1}$$

is a real bounded measurable function verifying the conditions:

$$\begin{gathered} v(q, q') = v(q', q) \\ |v(q, q')| \leqq V, \quad \forall q, q' \in \mathbb{R}^3\,. \end{gathered} \tag{5.2}$$

Let $\{\varphi_k\}$ be a complete orthonormal system in E. We write the one-particle density matrix in the form

$$T(q, q') = \sum_{k=1}^{\infty} \lambda_k\, \varphi_k(q)\, \overline{\varphi_k(q')}\,. \tag{5.3}$$

The positivity condition for the gauge-invariant quasi-free state defined by T implies [9, 10]

$$0 \leqq \lambda_k \leqq 1\,. \tag{5.4}$$

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

$$\sum_{k=1}^{\infty} \lambda_k < \infty\,. \tag{5.5}$$

$T(q, q')$ determines an operator $T \in H_1(E)$ such that

$$T\psi = \sum_{k=1}^{\infty} \lambda_k(\psi, \varphi_k)\varphi_k . \tag{5.6}$$

Of course

$$\|T\|_1 = \sum_{k=1}^{\infty} \lambda_k = \int_{\mathbb{R}^3} T(q, q)\, d^3 q . \tag{5.7}$$

We define

$$B_D(\cdot): H_1(E) \to H(E), \qquad B_{EX}(\cdot): H_1(E) \to H(E)$$

by the equalities

$$B_D(T)\varphi = U_D \varphi, \; B_{EX}(T)\varphi = U_{EX}\varphi \qquad \forall \varphi \in E \tag{5.8}$$

where U_D and U_{EX} are given by (1.2), (1.3) respectively.

It is easy to see that B_D is bounded and

$$|||B_D||| \leqq V . \tag{5.9}$$

Since

$$\begin{aligned} \|B_{EX}(T)\| &\leqq \left(\iint_{\mathbb{R}^3 \times \mathbb{R}^3} |v(q, q')\, T(q, q')|^2\, d^3 q\, d^3 q' \right)^{\frac{1}{2}} \\ &\leqq V \left(\sum_{k=1}^{\infty} \lambda_k^2 \right)^{\frac{1}{2}} \leqq V \|T\|_1 \end{aligned} \tag{5.10}$$

also $|||B_{EX}||| \leqq V$, so that $B(T) = B_D(T) + B_{EX}(T)$ satisfies the hypotheses of Section 2. Hence the existence theorem applies and Proposition 4.3 guarantees that $T(t)$, $t \in]0, \tau]$ satisfies the positivity condition (5.4) if T_0 satisfies (5.4). Hence $T(t)$ defines a quasi-free state. Furthermore the state remains pure if it is initially pure ($T_0^2 = T_0$).

The existence of the strong solution is guaranteed by the following condition on the initial state

$$R_T \subseteqq D_A . \tag{5.11}$$

This condition is physically reasonable in the greatest majority of the applications, where A is either the kinetic energy operator, or the kinetic energy plus a central field. If (5.11) holds, $A\,T_0$ is bounded so that Eq. (3.3) holds.

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