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

A. Bove

Istituto di Fisica dell'Università di Bologna, Bologna, Italy

G. Da Prato

Istituto Matematico "G. Castelnuovo" dell'Università di Roma, Roma, Italy

G. Fano

Istituto di Fisica dell'Università di Bologna, Bologna, Italy

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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: $\sup\limits_{q,q'}|v(q,q')|<+\infty$.

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:

$$T(t)x=e^{-itA}T_0e^{itA}x+i\int_0^t e^{-i(t-s)A}[T(s),B(T(s))]_-\,e^{i(t-s)A}x\,ds \tag{2.3}$$

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

$$\begin{cases} i\dfrac{dT(t)}{dt}x=A\,T(t)x-T(t)Ax+[B(T(t)),T(t)]_-x \\ T(0)x=T_0x\,. \end{cases} \tag{2.4}$$

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*

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

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:*

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

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

$$\|e^{-itA} T e^{itA}\|_1 = \|T\|_1. \qquad (3.6)$$

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

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

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

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

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*

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

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*

$$(x, y) \to \langle T_0 x, A y\rangle + \langle A x, T_0 y\rangle \qquad \forall (x, y) \in D_A \times D_A$$

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*

$$T(t) = e^{-iK(t)} T_0 e^{iK(t)} . \tag{4.4}$$

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

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

[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:

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

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

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

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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A. Bove
Istituto di Fisica
dell' Università
di Bologna
Via Irnerio 46
I-40126 Bologna, Italy