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The Time-dependent Hartree-Fock Equations with Coulomb Two-Body Interaction

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Abstract. The existence and uniqueness of global solutions to the Cauchy problem is proved in the space of "smooth" density matrices for the time-dependent Hartree-Fock equations describing the motion of finite Fermi systems interacting via a Coulomb two-body potential.

1. Introduction

In this note, we indicate how to generalize the recent results of Bove, Da Prato, and Fano [1] concerning the time-dependent Hartree-Fock equations with bounded two-body interaction to include the Coulomb two-body interaction. (See this work and the references therein for a discussion of the origin of the problem.) Specifically we consider the existence of global solutions to the Cauchy problem for the equations

$$idK/dt=[\tfrac{1}{2}\Delta - U, K]_- , \tag{1.1}$$

where $K=K(t)$ is a density matrix [i.e. a non-negative trace class operator on $L^2(R^3)$] and U is the self-consistent potential $U_D - U_{\text{EX}}$ defined by

$$(U_D f)(x)=\left(\int |x-y|^{-1}k(y, y; t)dy\right)f(x) \tag{1.2}$$

and

$$(U_{\text{EX}} f)(x)= -\int |x-y|^{-1}k(x, y; t)f(y)\,dy \tag{1.3}$$

when $K(t)$ is represented as the integral operator $(K(t)f)(x)=\int k(x, y; t)f(y)dy$. The idea of the argument is to extend to this situation our results [2] for N-electron systems governed by the Hartree-Fock equations

$$i\,\partial\varphi_j/\partial t=\tfrac{1}{2}\Delta\varphi_j - U_{\text{op}}\varphi_j , \tag{1.4}$$

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where

$$U_{\text{op}}\varphi_j(x,t)=\sum_{l=1}^{N}\Big(\varphi_j(x,t)\int|x-y|^{-1}|\varphi_l(y,t)|^2\,dy$$
$$-\varphi_l(x,t)\int|x-y|^{-1}\overline{\varphi}_l(y,t)\varphi_j(x,t)\,dy\Big). \tag{1.5}$$

The connection between the problems (1.1)–(1.3) and (1.4), (1.5) is the following: Suppose $\varphi_j(x,t)$ is the unique global solution of the latter Cauchy problem with data $\varphi_j(x,0)=\sqrt{\lambda_j}\varphi_j^0(x)$, then $k_N(x,y;t)=\sum_{j=1}^{N}\varphi_j(x,t)\overline{\varphi}_j(y,t)$ is the kernel of a solution of the original Cauchy problem with data K_N^0 having kernel $\sum_{j=1}^{N}\lambda_j\varphi_j^0(x)\overline{\varphi}_j^0(y)$. In this framework, the results of [2] can be interpreted as a solution of the problem (1.1)–(1.3) within a certain class of finite-rank operators. Section 2 of this paper consists of making precise this idea as well as that of taking the limit $N\to\infty$. The key ingredient in the limiting procedure will be the a priori estimates developed in Lemma 3.4 of [2].

2. The Results

It is well-known that in order to handle the Coulomb potential one must ultimately introduce derivatives (see, for example, the calculations of Lemma 2.3 of [2] which are typical). For this reason the solution space is taken to be the following Banach space of "smooth" operators.

Definition 2.1. Let A^2 denote the self-adjoint realization of $I-\Delta$ on $L^2(\mathbb{R}^3)$. Suppose $\mathscr{L}(L^2(\mathbb{R}^3))$ is the set of all bounded operators on $L^2(\mathbb{R}^3)$ and $\mathscr{L}^1(L^2(\mathbb{R}^3))$ is the set of trace class operators on $L^2(\mathbb{R}^3)$. Define $S=\{K;\,K\in\mathscr{L}(L^2(\mathbb{R}^3))$ and $A|K|A\in\mathscr{L}^1(L^2(\mathbb{R}^3))\}$ with the norm in S taken to be $\|K\|_{1,1}=\operatorname{tr}(A|K|A)=\|A|K|A\|_1$.

In what follows we use $\|\cdot\|$ to denote the norm in $L^2(\mathbb{R}^3)$ and $\mathscr{L}(L^2(\mathbb{R}^3))$, $\|\cdot\|_1$ the norm in $\mathscr{L}^1(L^2(\mathbb{R}^3))$ and $\|\cdot\|_{1,1}$ for the norm in S in as much as it corresponds to the Sobolev space $H^1(\mathbb{R}^3)$ of scalar functions. Indeed for physical reasons we are only interested in the cone of positive operators in S, denoted by S^+ and called smooth density matrices. Before beginning the main discussion, we summarize some ideas about trace class operators (cf. [3]) which will be useful in the later calculations. Since $|K|\geqq 0$, then $A|K|A\geqq 0$ so that $\|K\|_{1,1}=\operatorname{tr}(A|K|A)=\|A|K|A\|_1$. But A^{-1} is bounded on $L^2(\mathbb{R}^3)$ so that $|K|=A^{-1}A|K|AA^{-1}$ and hence $K\in\mathscr{L}^1(L^2(\mathbb{R}^3))$. Thus K can be written as an integral operator $(Kf)(x)=\int k(x,y)f(y)dy$, with kernel $k(x,y)\in L^2(\mathbb{R}^3)\times L^2(\mathbb{R}^3)$ and $|k|(x,x)\in L^1(\mathbb{R}^3)$. Moreover $k(x,y)=\sum_{j=1}^{\infty}\lambda_j\varphi_j(x)\overline{\varphi}_j(y)$ and the kernel associated with $|K|$, $|k|(x,y)=\sum_{j=1}^{\infty}|\lambda_j|\varphi_j(x)\overline{\varphi}_j(y)$ [where $\{|\lambda_j|,\varphi_j\}$ is a spectral set for $|K|$ and the convergence is in $L^2(\mathbb{R}^3)\times L^2(\mathbb{R}^3)$ with $\sum|\lambda_j|=\sum|\lambda_j|\,\|\varphi_j\|^2=\int|k|(x,x)dx<\infty$]. Finally, because $|K|\varphi_j=|\lambda_j|\varphi_j$, $A\varphi_j=|\lambda_j|^{-1}A|K|\varphi_j=|\lambda_j|^{-1}A|K|AA^{-1}\varphi_j$. Thus $\|A\varphi_j\|\leqq|\lambda_j|^{-1}\|A|K|A\|\,\|A^{-1}\varphi_j\|\leqq|\lambda_j|^{-1}\|A|K|A\|_1\|\varphi_j\|=|\lambda_j|^{-1}\|K\|_{1,1}$, so that $\varphi_j\in D(A)$. Thus the kernel of $A|K|A$ is $\sum|\lambda_j|A\varphi_j(x)\overline{A\varphi_j}(y)$ and $\|K\|_{1,1}=\sum|\lambda_j|\,\|A\varphi_j\|^2$.

Definition 2.2. $K(t)$ is a solution of the Cauchy problem (1.1)–(1.3) over the interval $(0, T)$ if the map $t \to K(t) : (0, T) \to S$ is continuous and $K(t)$ satisfies the integrated form of Eq. (1.1),

$$K(t) = e^{-i\Delta/2t} K(0) e^{i\Delta/2t} + i \int_0^t e^{-i\Delta/2(t-s)} [U, K](s) e^{i\Delta/2(t-s)} ds\,, \tag{2.1}$$

the last integral being interpreted in the strong Riemann sense in S.

Proposition 2.3. *The Eq.* (2.1) *has a unique local solution in* S.

Proof. Segal's generalization of the Picard-Lipschitz theory to infinite dimensional spaces [4, p. 343, Theorem 1] can be applied directly. First the free propagator is a contraction group since $\|e^{-i\Delta/2t} K e^{i\Delta/2t}\|_{1,1} = \|A|e^{-i\Delta/2t} K e^{i\Delta/2t}|A\|_1 = \|Ae^{-i\Delta/2t}|K|e^{i\Delta/2t}A\| = \|e^{-i\Delta/2t}A|K|Ae^{i\Delta/2t}\|_1$ by the spectral theorem and the last equals $\|A|K|A\|_1 = \|K\|_{1,1}$ by [1, p. 186, Proposition 3.4]. The local Lipschitz nature of the non-linearity follows essentially as usual. By straightforward algebra

$$[U(T), T] - [U(S), S] = [U(T), T-S] - [U(T-S), S]\,,$$

so that it is enough to show that $\|U(K)L\|_{1,1}$ and $\|LU(K)\|_{1,1} \leqq C\|K\|_{1,1}\|L\|_{1,1}$. Now $\|U(K)L\|_{1,1} = \mathrm{tr}(A|U(K)L|A) = \mathrm{tr}(|U(K)L|A^2) \leqq \|U(K)\|\ \|K\|_1$ extracting the partial isometries in the polar decomposition of $U(K)$ and $U(K)L$ from the left. Similarly $\|LU(K)\|_{1,1} = \mathrm{tr}(A^2|LU(K)|) \leqq \|L\|_{1,1}\|U(K)\|$. Thus one must show that $\|U_D(K)\|$ and $\|U_{\mathrm{EX}}(K)\| \leqq \text{const}\ \|K\|_{1,1}$. This follows directly from the Sobolev type estimates in [2, Lemma 2.3].

Suppose K has a kernel $\sum \lambda_j \psi_j(x)\overline{\varphi}_j(y)$ where $\{|\lambda_j|, \varphi_j\}$ is a spectral set for $|K|$ and $\{\psi_j\}$ is an orthonormal basis in $L^2(\mathbb{R}^3)$. $U_D(K)$ is multiplication by $\sum \lambda_j \int |x-y|^{-1}\psi_j(y)\overline{\varphi}_j(y)dy$ and so

$$\begin{aligned}
\|U_D(K)\| &\leqq \sum |\lambda_j| \sup_x \int |x-y|^{-1}|\psi_j(y)|\ |\varphi_j(y)|dy \\
&\leqq \sum |\lambda_j|\ \|\psi_j\|\ \|\int |x-y|^{-1}|\varphi_j(y)|dy\| \\
&\leqq C \sum |\lambda_j|\ \|\nabla \varphi_j\| \\
&\leqq C \sum |\lambda_j|^{\frac{1}{2}}(|\lambda_j|\ \|\nabla\varphi_j\|^2)^{\frac{1}{2}} \\
&\leqq \tfrac{1}{2} C \sum |\lambda_j|(1 + \|\nabla\varphi_j\|^2) = \tfrac{1}{2} C\,\|K\|_{1,1}\,.
\end{aligned}$$

For the exchange term,

$$\begin{aligned}
\|U_{\mathrm{EX}}(K)f\| &= \|\int \sum \lambda_j |x-y|^{-1}\psi_j(x)\overline{\varphi}_j(y)f(y)dy\| \\
&\leqq \sum |\lambda_j|\ \|\psi_j\| \sup_x \int |x-y|^{-1}|\varphi_j(y)|\ |f(y)|dy \\
&\leqq C \sum |\lambda_j|\ \|\nabla\varphi_j\|\ \|f\| \\
&\leqq \tfrac{1}{2} C\,\|K\|_{1,1}\|f\|\,.
\end{aligned}$$

The fact that if K at $t=0$ is positive it remains positive in the interval of existence is proved in [1].

In proving that this solution can be extended to all of $(0, \infty)$ we shall make use of the following representation of finite rank solutions in S^+.

Proposition 2.4. *Suppose the initial data K^0 is a finite rank operator in S^+; i.e. $K^0 = \sum_{j=1}^{N} \lambda_j \varphi_j^0(x)\overline{\varphi_j^0}(y)$ where $\{\lambda_j \geqq 0, \varphi_j^0\}_{j=1}^N$ is a spectral set in $L^2(\mathbb{R}^3)$ with $\varphi_j^0 \in D(A) \cong H^1$ for all $j=1, \ldots, N$. Denote by $\varphi_j(x,t)$, $j=1,2,\ldots N$ the unique (global) solution of the (integral form of) Eq. (1.4) in $H^1(\mathbb{R}^3)$ with initial data $\sqrt{\lambda_j}\, \varphi_j^0(x)$ as given in [2]. Then*

$$K(t) = \sum_{j=1}^{N} \varphi_j(x,t)\overline{\varphi_j}(y,t) = \sum_{j=1}^{N} \lambda_j(\varphi_j(x,t)/\sqrt{\lambda_j})\,(\overline{\varphi_j}(y,t)/\sqrt{\lambda_j})$$

is the unique global solution in S^+ of (the integral form of) problem (1.1)–(1.3) *with initial data K^0.*

Proof. The idea of the proof can be seen most easily from the viewpoint of the differential equations and the proof for the integral equations involves only simple but non-essential algebraic considerations. From (1.4)

$$\begin{aligned} i\partial\varphi_j(x,t)/\partial t\,\overline{\varphi_j}(y,t) &= \tfrac{1}{2}\Delta\varphi_j(x,t)\overline{\varphi_j}(y,t) - \sum_{l=1}^{N} \varphi_j(x,t)\overline{\varphi_j}(y,t) \int |x-z|^{-1}|\varphi_l(z,t)|^2\, dz \\ &\quad + \sum_{l=1}^{N} \varphi_l(x,t)\overline{\varphi_j}(y,t) \int |x-z|^{-1}\overline{\varphi_l}(z,t)\varphi_j(z,t)\, dz\,. \end{aligned}$$

Taking conjugates, exchanging x and y, adding the new equation to the above and summing over j from l to N one obtains

$$\begin{aligned} i\,\partial/\partial t \sum_{j=1}^{N} \varphi_j(x,t)\overline{\varphi_j}(y,t) &= \tfrac{1}{2}\Big(\sum_j \Delta\varphi_j(x,t)\varphi_j(y,t) - \sum_j \varphi_j(x,t)\overline{\Delta\varphi_j}(y,t)\Big) \\ &\quad - \int \Big(|x-z|^{-1} \sum_j \varphi_j(x,t)\overline{\varphi_j}(y,t) \sum_l \varphi_l(z,t)\overline{\varphi_l}(z,t) \\ &\quad - |y-z|^{-1} \sum_j \varphi_j(x,t)\overline{\varphi_j}(y,t) \sum_l \varphi_l(z,t)\overline{\varphi_l}(z,t)\Big)\, dz\,, \\ &\quad + \int \Big(|x-z|^{-1} \sum_j \varphi_j(z,t)\overline{\varphi_j}(y,t) \sum_l \varphi_l(x,t)\overline{\varphi_l}(z,t) \\ &\quad - |y-z|^{-1} \sum_j \varphi_j(x,t)\overline{\varphi_j}(z,t) \sum_l \varphi_l(z,t)\overline{\varphi_l}(y,t)\Big)\, dz\,, \end{aligned}$$

which is just Eq. (1.1) written for the kernel $\sum_j \varphi_j(x,t)\overline{\varphi_j}(y,t)$. From [2, Lemmas 3.1 and 3.4] $\|\varphi_j(t)/\sqrt{\lambda_j}\| = \|\varphi_j^0\| = 1$ and $\varphi_j(t) \in D(A)$ for all t. One can also show in the same manner that since the $\{\varphi_j^0\}$ are orthogonal, the $\{\varphi_j(t)\}$ are orthogonal for each t. Thus $K(t) = \sum \lambda_j(\varphi_j(x,t)/\sqrt{\lambda_j})\,(\overline{\varphi_j}(y,t)/\sqrt{\lambda_j})$ is the unique global solution of (1.1) in S^+ with the given Cauchy data.

Theorem 2.5. *The Cauchy problem for (the integral version of) the Eq.* (1.1) *has a unique global solution in S^+.*

Proof. Suppose the Cauchy data at $t=0$ is $K^0 = \sum_{j=1}^{\infty} \lambda_j \varphi_j^0(x)\overline{\varphi_j^0}(y)$ where, since $K^0 \in S^+$, $\{\lambda_j \geqq 0, \varphi_j^0\}$ is a spectral set and $\|K^0\|_{1,1} = \sum_{j=1}^{\infty} \lambda_j(1 + \|\nabla\varphi_j^0\|^2) < \infty$.

Then $\left\{K_N^0 = \sum_{j=1}^{N} \lambda_j \varphi_j^0(x)\overline{\varphi_j^0(y)}\right\}_{N=1}^{\infty}$ is a sequence of finite rank operators approximating K^0 in S. From the above $K_N(t) = \sum_{j=1}^{N} \lambda_j(\varphi_j(x,t)/\sqrt{\lambda_j})(\overline{\varphi_j}(y,t)/\sqrt{\lambda_j})$ is the unique global solution of Eq. (1.1) with data K_N^0 at $t=0$. The theorem will be proved if we can show that for each $t \in (0,\infty)$, $K_N(t)$ converges in S (indeed, we will show that the convergence is uniform in t) and that the limiting operator function of t is a solution of (1.1).

To this end consider, for any $t \in (0,\infty)$,

$$\begin{aligned}\|K_N(t)-K_M(t)\|_{1,1} &= \sum_{j=M}^{N} \lambda_j(\|\varphi_j(t)/\sqrt{\lambda_j}\|^2 + \|\nabla\varphi_j(t)/\sqrt{\lambda_j}\|^2)\\ &= \sum_{j=M}^{N} \lambda_j(1+\lambda_j^{-1}\|\nabla\varphi_j(t)\|^2)\\ &= \sum_{j=M}^{N} \lambda_j + \sum_{j=M}^{N} \|\nabla\varphi_j(t)\|^2,\end{aligned}$$

where we have used the estimate [2, Lemma 3.1] $\|\varphi_j(t)/\sqrt{\lambda_j}\| = \|\varphi_j^0\| = 1$. From [2, Lemma 3.4], since $\varphi_j(t)$ is a solution of (1.4),

$$\sum_{j=1}^{N} \|\nabla\varphi_j(t)\|^2 + \sum_{j=1}^{N}\sum_{l=1}^{N} I_{j,l}(t) = \sum_{j=1}^{N} \|\nabla\varphi_j(0)\|^2 + \sum_{j=1}^{N}\sum_{l=1}^{N} I_{j,l}(0), \tag{2.2}$$

where $I_{j,l}(t) = \int v_l(x,t)|\varphi_j(x,t)|^2 - 1/4\pi|\nabla v_{jl}(x,t)|^2 dx$, with $v_l(x,t)$ and $v_{j,l}(x,t)$ being respectively the first and second integral in Eq. (1.5). Now $I_{j,l}(t) \geqq 0$ (cf. [2], from Eq. (3.7) on) for each j, l, so that

$$\begin{aligned}\sum_{j=M}^{N} \|\nabla\varphi_j(t)\|^2 &\leqq \sum_{j=N}^{N} \|\nabla\varphi_j(0)\|^2 + \sum_{j=1}^{N}\sum_{l=1}^{N} I_{j,l}(0) - \sum_{j=1}^{M}\sum_{l=1}^{M} I_{j,l}(0)\\ &\leqq \sum_{j=M}^{N} \lambda_j\|\nabla\varphi_j^0\|^2 + \sum_{j=M}^{N}\sum_{l=1}^{M} I_{j,l}(0) + \sum_{j=1}^{N}\sum_{l=M}^{N} I_{j,l}(0).\end{aligned}$$

But $I_{j,l}(0) = \int \{(\int |x-y|^{-1}|\varphi_l(x,0)|^2 dy)\,|\varphi_j(x,0)|^2 - 1/4\pi|\nabla \int |x-y|^{-1}\overline{\varphi_l}(y,0)\varphi_j(y,0)\cdot dy|^2\}dx$, so that

$$\begin{aligned}I_{j,l}(0) &\leqq \lambda_j\lambda_l\left(\sup_x \int |x-y|^{-1}|\varphi_l^0(y)|^2 dy\,\|\varphi_j^0\|^2 + 1/4\pi\|\int |x-y|^{-2}|\varphi_l^0(y)|\,|\varphi_j^0(y)|dy\|^2\right)\\ &\leqq \lambda_j\lambda_l(2\|\varphi_l^0\|\,\|\varphi_j^0\|^2\,\|\nabla\varphi_l^0\| + c/4\pi\|\varphi_l^0\varphi_j^0\|_{6/5}^2)\\ &\leqq C\lambda_j\lambda_l(\|\varphi_l^0\|\,\|\nabla\varphi_l^0\|\,\|\varphi_j^0\|^2 + \|\varphi_l^0\|_{12/5}^2\|\varphi_j^0\|_{12/5}^2)\\ &\leqq C\lambda_j\lambda_l(\|\varphi_l^0\|\,\|\nabla\varphi_l^0\|\,\|\varphi_j^0\|^2 + \|\nabla\varphi_l^0\|^{1/2}\|\varphi_l^0\|^{3/2}\|\nabla\varphi_j^0\|^{1/2}\|\varphi_j^0\|^{3/2})\\ &\leqq C\lambda_j\lambda_l(\|\varphi_l^0\|^2 + \|\nabla\varphi_l^0\|^2)(\|\varphi_j^0\|^2 + \|\nabla\varphi_j^0\|^2),\end{aligned}$$

where we have used Sobolev inequalities as they appear in [5, p. 220] and [6, p. 27, Theorem 10.1] in a manner like [2] and the inequality $a^{1/l}b^{1/m} \leqq a/l + b/m$ if $1/l + 1/m = 1$. The constant C changes from line to line. Thus

$$\|K_N(t)-K_M(t)\|_{1,1} \leqq C(1+\|K^0\|_{1,1})\,\|K_N^0 - K_M^0\|_{1,1}$$

showing that $\{K_N(t)\}$ is Cauchy in S uniformly in $t\in(0,\infty)$ since $K_N^0\to K^0$ in S. As a result $\{K_N(t)\}$ converges in S uniformly in $t\in(0,\infty)$ to an operator which is continuous in $t\in(0,\infty)$ [since for each N, $K_N(t)$ is continuous in S] and positive. The uniformity in t of the convergence, the continuity of the non-linearity in S and the invariance of the $\|\cdot\|_{1,1}$-norm under the free motion (Proposition 2.3) guarantee that the limiting operator is a solution of Eq. (2.1) in S. Thus it is the (necessarily unique) global solution of the Cauchy problem in S^+ of Eq. (1.1)–(1.3).

In conclusion we remark that other two body potentials (e.g. Yukawa) along with the inclusion of a central potential can be treated in this manner by suitably adjusting the "Sobolev spaces" $S_{n,p}=\{K\in\mathscr{L}(L^2(\mathbb{R}^3)), \|K\|_{n,p}^p=\mathrm{tr}(A^n|K|^pA^n)<\infty\}$ in a manner suggested by the classical (i.e. scalar or vector) theory of partial differential equations.

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