Local well-posedness for the evolution of relativistic electrons coupled with a classical nucleus

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Framework

We consider a system of 2 electrons represented by a wave function $\psi : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{C}^{16}$ and evolving according in the field of one nucleus in position $q(t)$ according to the energy :

$$\mathcal{E} = \frac{1}{2} \sum_{j=1,2} \int \langle \psi D_j, \psi \rangle + \frac{1}{2} Z \sum_{j=1,2} \int \langle \psi, \frac{1}{x_j - q(t)} \psi \rangle - \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} |x_1 - x_2|^{-1} \langle \psi, \psi \rangle.$$

$D_j = m\beta + i\vec{\alpha} \cdot \nabla_j$: Dirac operator associated to the variable x_j.
$\langle \cdot, \cdot \rangle$: either the canonical product on $\mathbb{C}^4 \otimes \mathbb{C}^4$ or $(\cdot, \beta \otimes \beta \cdot)$.
In the sequel, we write $\overline{\psi}_1 \psi_2$ for $\langle \psi_1, \psi_2 \rangle$.

Ansatz

Since the electrons are fermions, they satisfy Pauli's principle, which means

$$\psi(x_1, x_2) = -\psi(x_2, x_1).$$

We take ψ to be equal to

$$\psi = \frac{1}{\sqrt{2}}(u_1(x_1) \otimes u_2(x_2) - u_1(x_2) \otimes u_2(x_1))$$

with $u_i : \mathbb{R}^3 \to \mathbb{C}^4$ orthogonal and normalised (Slater determinant).

Ansatz 2

We get the following energy :

$$\mathcal{E} = \mathcal{E}_{kin} + \mathcal{E}_{pot} + \mathcal{E}_{mf} + \mathcal{E}_{exch}$$

with

$$\begin{aligned}
\mathcal{E}_{kin} &= \frac{1}{2}\sum_j \int \overline{u}_j D u_j \\
\mathcal{E}_{pot} &= \frac{Z}{2}\sum_j \int \overline{u}_j |x - q(t)|^{-1} u_j \\
\mathcal{E}_{mf} &= -\frac{1}{2}\int \Big(|x|^{-1} * |u_1|^2\Big)|u_2|^2 \\
\mathcal{E}_{exch} &= -\frac{1}{2}\int \Big(|x|^{-1} * (\overline{u}_1 u_2)\Big)\overline{u}_2 u_1 .
\end{aligned}$$

A system of equations

$$
\begin{aligned}
i\partial_t u_1 &= Du_1 + Z|x-q(t)|^{-1}u_1 - |x|^{-1} * |u_2|^2 u_1 - |x|^{-1} * (u_1\overline{u}_2)u_2 \\
i\partial_t u_2 &= Du_2 + Z|x-q(t)|^{-1}u_2 - |x|^{-1} * |u_1|^2 u_2 - |x|^{-1} * (u_2\overline{u}_1)u_1.
\end{aligned}
$$

For the sake of simplicity, we solve

$$i\partial_t u = Du + |x-q(t)|^{-1}u + |x|^{-1} * |u|^2 u.$$

What is important is that the local (in time) analysis is not so much affected (depending on the results we wish to prove).

The equation on q

The nucleus, because it is heavy compared to the electrons, is supposed to behave in a classical way. It is in the field of the electrons, which means that it potential energy is

$$E_{pot,n} = \int \overline{u}|x - q(t)|^{-1} u$$

from which we get the coupling

$$Mq''(t) = -\nabla_q \int \overline{u}|x - q(t)|^{-1} u = 3 \int \overline{u} \frac{x - q(t)}{|x - q(t)|^3} u.$$

Previous works

The non-relativistic equivalent of this equation :

$$\begin{cases} i\partial_t u = -\triangle u + Z|x-q(t)|^{-1}u + |x|^{-1} * |u|^2 u \\ Mq''(t) = -\nabla_q \int \overline{u}|x-q(t)|^{-1}u \end{cases}$$

was studied by Cancès and Lebris '99, they prove global well-posedness in $\mathcal{C}(\mathbb{R}, H^2) \times \mathcal{C}(\mathbb{R}^2)$. The GWP is based on energy conservation and H^2 estimates.

The linear problem $i\partial_t u = -\triangle u + |x-q(t)|^{-1}u$ with fixed $q(t)$ was studied by Kato and Yajima, '91, in an ever more refined way, with retarded time approximation (take $q(s(t))$ instead of $q(t)$).

Result

Theorem [F.Cacciafesta, D. Noja, dS] We assume Z is small enough. There exists C_1 and C_2 depending on Z, such that for all $R \in \mathbb{R}_+$, all $u_0 \in H^2$ such that $\|u_0\|_{H^1} \leq R$, and all q_0' such that $|q_0'| \leq C_1$, the above equation with initial data $q(0) = 0$, $q'(0) = q_0'$ and $u(0) = u_0$ is well-posed in $\mathcal{C}([0, T], H^2(R^3)) \times C^2([0, T]$, for $T \leq \frac{1}{C_2 R^2}$.

We remark that the equation scales with critical regularity $s_c = 0$. This means that we should get better results for the time of existence. Nevertheless, the restriction on the regularity of the initial datum is due to the coupling and it seems difficuly to lower it.

Change of variables

We study $i\partial_t u = Du + Z|x - q(t)|^{-1}u$. With the change of variable $v(t) = I(t)u(t) = u(t, x + q(t))$, we get

$$i\partial_t v = Dv + Z|x|^{-1}v + iq'(t) \cdot \nabla v.$$

If Z and $\|q'\|_{L^\infty([0,T])}$ are small enough then the operator $H(t) = D + Z|x|^{-1} + iq'(t) \cdot \nabla$ satisfies for all $t \in [0, T]$

$$\frac{1}{C}\|v\|_{H^1} \leq \|H(t)v\|_{L^2} \leq C\|v\|_{H^1}.$$

Linear Analysis in L^2

Theorem [Kato, '52] Assume that for all time $t \in [0, T]$, $H(t)$ is a continuous in time, $\mathcal{L}(H^1, L^2)$ essentially self-adjoint operator, then the propagator $U(t, s)$ of the equation $i\partial_t u = H(t)u$ exists and belongs to $\mathcal{C}([0, T], \mathcal{L}(L^2)$ and $\|U(t, s)\|_{L^2 \to L^2} \leq 1$.
What is more $U(t, s)$ is the limit when N goes to ∞ of

$$\prod_{k=1}^{N} e^{i(t_k - t_{k-1})H(t_{k-1})}$$

with $t_0 = s, h = \frac{t-s}{N}, t_k = t_0 + hk$.

Linear analysis in H^m

From the previous theorem, we know that the linear equation is well-posed in L^2 but we would like some more regularity. Assume $v \in \mathcal{C}([0, T], H^m)$ and write $w(t) = H(t)^m v(t)$ for some positive integer m. The fact that v solves $i\partial_t v = H(t)v$ is equivalent to the fact that w solves

$$i\partial_t w = H(t)w + i \sum_k H(t)^k H'(t) H(t)^{1-k}(t)w.$$

This means

$$w(t) = U(t, t_0)w(t_0) + i \int_{t_0}^{t} U(t, s) \sum_k H(s)^k q''(s) \cdot \nabla H(t)^{1-k}(s)w(s)ds.$$

Linear Analysis in H^m

With $\|q''\|_{L^1([0,T])}$ small enough, this is well posed in L^2.

We get $w(t) = V(t,s)w(s)$ with $V \in \mathcal{C}([0,T]^2, \mathcal{L}(L^2))$.

We have $v(t) = H(t)^{-1}V(t,s)H(s)v(s)$ with the propagator $H(t)^{-1}V(t,s)H(s)$ in $\mathcal{C}([0,T]^2, \mathcal{L}(H^m))$.

And finally $u(t) = I(t)^{-1}H(t)^{-1}V(t,s)H(s)I(s)u(s)$ with the propagator $U_q(t,s)$ in $C([0,T]^2, \mathcal{L}(H^m))$.

Dependance on q

We have $\|H_{q_1}(t) - H_{q_2}(t)\|_{H^m \to H^{m-1}} \lesssim \|q_1' - q_2'\|_{L^\infty([0,T]}$ for all $t \in [0, T]$.
What is more, $I_q(t)U_q(t,s)I_q(s)^{-1}$ is the limit of

$$\prod_{k=1}^{N} e^{i(t_k - t_{k-1})H_q(t_{k-1})}$$

Hence

$$\|U_{q_1}(t,s) - U_{q_2}(t,s)\|_{H^m \to H^{m-1}} \leq \|q_1' - q_2'\|_{L^\infty([0,T])}.$$

Linear analysis- Result

Proposition [Cacciafesta, Noja, dS] Assuming that Z, $\|q'\|_{L^\infty}$ and $\|q''\|_{L^1}$ are small enough, the propagator U_q of the equation $i\partial_t u = H_q(t)u$ belongs to $\mathcal{C}([0,T]^2, H^m)$ for all $m \in \mathbb{N}$.
What is more, and under the same assumptions for q_1 and q_2 (with $q_1(0) = q_2(0) = 0$), for $m \in \mathbb{N}^*$, we have

$$\|U_{q_1}(t,s) - U_{q_2}(t,s)\|_{H^m \to H^{m-1}} \leq \|q_1' - q_2'\|_{L^\infty([0,T])}.$$

Contraction in H^2

Fixing $q(t)$, the equation on u, is written

$$u(t) = U_q(t,t_0)u_0 - i\int_{t_0}^{t} U_q(t,s)|x|^{-1} * |u|^2(s)u(s)ds.$$

Thanks to Hardy inequality, we have,

$$\||x|^{-1} * |u|^2(s)u(s)\|_{H^j} \lesssim \|u(s)\|_{H^j}\|u\|_{H^1}^2$$

and

$$\||x|^{-1}*|u|^2(s)u(s)-|x|^{-1}*|v|^2(s)v(s)\|_{H^1} \lesssim \|u(s)-v(s)\|_{L^2}(\|u\|_{H^1}^2+\|v\|_{H^1}^2).$$

This enables us to perform a contraction argument in H^2, we get a flow $\Psi_q(t)$ which satifies for $t \in [0, T \sim \frac{1}{\|u_0\|_{H^1}^2}]$,

$$\|(\Psi_{q_1}(t) - \Psi_{q_2}(t))u_0\|_{L^\infty([0,T],H^1)} \lesssim \|q_1' - q_2'\|_{L^\infty([0,T])}\|u_0\|_{H^2}.$$

Contraction for q

We now proceed to a contraction argument on q. We solve the fix point

$$Mq(t) = tq_0' + 3\int_{t_0}^{t}\int_{t_0}^{\tau}\int \overline{\Psi_q(s)u_0}(x - q(t))|x - q(s)|^{-3}\Psi_q(s)u_0 ds d\tau.$$

We have

$$\Big|\int \overline{(\Psi_{q_1}(t)u_0 - \Psi_{q_2}(t)u_0)}(x - q_1(t))|x - q_1(t)|^{-3}\Psi_{q_1}(t)u_0\Big| \lesssim \|\Psi_{q_1}(t)u_0 - \Psi_{q_2}(t)u_0\|_{H^1}\|\Psi_{q_1}(t)u_0\|_{H^1}.$$

Contraction for q, 2

For a fixed u, setting

$$F(q) = \int \overline{u}|x-q|^{-3}(x-q)u = \int \overline{u_q}x|x|^{-3}u_q$$

where $u_q(x) = u(x+q)$, we have

$$\nabla F = 2\mathrm{Re} \int \overline{(\nabla u)_q} x|x|^{-3}u_q.$$

We get

$$|\nabla F| \leq ||u||_{H^2}||u||_{H^1}.$$

For these reasons, one can proceed to a contraction argument for times of order $\frac{1}{||u_0||_{H^2}||u_0||_{H^1}}$.

Schauder fix point

Assume A is a map from $C^1([0,T])$ to itself and that K is a compact of $\mathcal{C}^1([0,T])$ such that $A(K) \subset K$. Then A admits a fix point in K. Note that the fix point is not unique.
Take $K(T) = \{q \in \mathcal{C}^2([0,T]) | q(0) = 0, \|q'\|_{L^\infty} \leq C_1, T\|q''\|_{L^\infty} \leq C_2\}$.
$K(T)$ is compact in $\mathcal{C}^1([0,T])$. The map

$$A(q) = tq_0' + 3\int_{t_0}^{t}\int_{t_0}^{\tau}\int \overline{\Psi_q(s)u_0}(x - q(t))|x - q(s)|^{-3}\Psi_q(s)u_0 ds d\tau$$

is continuous on $K(T)$ as long as u_0 is in H^2 but with no restriction on the norm and

$$A(K(T)) \subseteq K(T)$$

as long as T is of order $\frac{1}{\|u_0\|_{H^1}^2}$.

Schauder fix point 2

There exists a fix point for the equation on q which enables us to define $u = \Psi_q(t)u_0$ for times of order $\frac{1}{\|u_0\|_{H^1}^2}$.

The uniqueness comes from the contraction on times of order $\frac{1}{\|u_0\|_{H^1}\|u_0\|_{H^2}}$.

Model

There is a model with multiple nuclei. In this case, the equation on u remains the same except that the potential term is now

$$\sum_j |x - q_j(t)|^{-1} u.$$

The equation on the different qs however must include the interaction between the nuclei. Hence

$$Mq_j'' = -Z_j \nabla_{q_j} \Big(\int \overline{u} |x - q_j(t)|^{-1} u - \sum_{k \neq j} Z_j Z_k |q_j - q_k|^{-1} \Big).$$

Linear Analysis

To deal with this new potential one has to introduce a change of variable that depends of which nucleus one is close to :

$$\Phi(t)x = x + \sum_j \eta(x - q_j)q_j(t)$$

where q_j are the id for $q_j(t)$.
This complicate things a little bit because things that were isometries like $I(t)$ lose this property.
It also enforces to take $q_j(t)$ that are well separated : at all times $|q_j(t) - q_k(t)| \geq \varepsilon_0 > 0$.
Write

$$H(t) = D + \sum_j |x - q_j(t)|^{-1}.$$

Linear analysis, Result

Proposition [Cacciafesta, Noja, dS] Assume that for all times in $[0, T]$, $|q_j(t) - q_k(t)| \geq \varepsilon_0 > 0$ and moreover that

$$\sum_{k=1}^{N} |Z_k| \leq C_Z \varepsilon_0$$

and

$$\sup_{k,t} |\dot{q}_k(t)| \leq \min(C_1, C_1 \frac{\varepsilon_0}{T}), \quad \sup_{k} \|\ddot{q}_k(t)\|_{L^1} \leq C_2,$$

for some suitably small positive constants C_1, C_2 and C_Z. Then the propagator of the equation

$$i\partial_t u = H(t)u$$

is a family of operators $U_q(t, s)$ with

$$U_q \in \mathcal{C}([0, T]^2, \mathcal{L}(L^2)) \cap \mathcal{C}([0, T]^2, \mathcal{L}(H^1)) \cap \mathcal{C}([0, T]^2, \mathcal{L}(H^2))$$

with norms uniformly bounded in q.

Linear analysis, Result

What is more, if $q^{(1)} = (q_1^{(1)}, \dots, q_N^{(1)})$ and $q^{(2)} = (q_1^{(2)}, \dots, q_N^{(2)})$ are two vectors of $\mathcal{C}^2([0,T])$ satisfying the same assumptions as q, and assuming that $q^{(1)}(0) = q^{(2)}(0)$, then there exists C_T such that for all $t, s \in [0,T]^2$, we have

$$
\|U_{q^{(1)}} - U_{q^{(2)}}\|_{H^m \to L^{m-1}} \leq
$$

$$
C_T \sup_{k,t} T \frac{|(\dot{q}_k{}^{(1)}) - (\dot{q}_k{}^{(2)})|}{\varepsilon_0} + C_T \sup_{k,t} |(\dot{q}_k{}^{(1)})(t) - (\dot{q}_k{}^{(2)})(t)|.
$$

Local well-posedness, Result

Theorem [Cacciafesta, Noja, dS] We assume $\sum_j Z_j \lesssim \varepsilon_0$. There exists C_1 and C_2 depending on $(Z_j)_j$, such that for all $R \in \mathbb{R}_+$, all $u_0 \in H^2$ such that $\|u_0\|_{H^1} \leq R$, and all vectors q_0' such that $|q_0'| \leq C_1$ and q_0 satisfying the well-separated assumption, the above equation with initial data $q(0) = q_0$, $q'(0) = q_0'$ and $u(0) = u_0$ is well-posed in $\mathcal{C}([0,T], H^2(\mathbb{R}^3)) \times C^2([0,T]$, for $T \leq \frac{\varepsilon_0^2}{C_2 R^2}$.