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Dirac equations with moving nuclei

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ABSTRACT. — A time dependent Dirac equation

$$\partial_t u + i(\alpha \cdot \mathrm{D} + (\varphi - \alpha \cdot \mathrm{A}) + m\beta) u = 0$$

is considered, where (A, φ) is the Liénard-Wiechert potential produced by a finite number of nuclei with charges Z_k moving along the trajectories $x = q_k(t)$, $k = 1, \ldots, \mathrm{N}$. We show that the equation uniquely generates a unitary propagator $\mathrm{U}(t, s)$ in $\mathrm{L}^2(\mathbb{R}^3, \mathbb{C}^4)$ such that $\mathrm{U}(t, s)\mathrm{H}^{\pm 1}(\mathbb{R}^3, \mathbb{C}^4) = \mathrm{H}^{\pm 1}(\mathbb{R}^3\ \mathbb{C}^4)$. The assumptions are: $|Z_k| < \sqrt{3}/2$ (or $\leqq 118$ in atomic units), $q_k \in \mathrm{C}^3$, $q_k(t) \neq q_j(t)$ for $k \neq j$ and $|\dot{q}_k(t)| \leqq v < 1$, $j, k = 1, \ldots, \mathrm{N}$. The proof uses a linear transformation of the unknown u associated with a "local pseudo-Lorentz transformation", which locally freezes the motion of the nuclei, and the theory of abstract evolution equations.

RÉSUMÉ. — Nous considérons une équation de Dirac qui dépend du temps $\partial_t u + i(\alpha \cdot \mathrm{D} + (\varphi - \alpha \cdot \mathrm{A}) + m\beta) u = 0$ où (A, φ) est le potentiel de Liénard-Wiechert produit par un nombre fini de nucléons de charge Z_k qui se déplacent sur des trajectoires $x = q_k(t)$, $k = 1, \ldots, \mathrm{N}$. Nous prouvons que l'équation engendre un unique propagateur $\mathrm{U}(t, s)$ dans $\mathrm{L}^2(\mathbb{R}^2, \mathbb{C}^4)$ tel que $\mathrm{U}(t, s)\mathrm{H}^{\pm 1}(\mathbb{R}^3, \mathbb{C}^4) = \mathrm{H}^{\pm 1}(\mathbb{R}^3, \mathbb{C}^4)$. Nous supposons que : $|Z_k| < \sqrt{3}/2$ (ou $\leqq 118$ en unités atomiques), $q_k \in \mathrm{C}^3$, $q_k(t) \neq q_j(t)$ pour $k \neq j$ et $|q_k(t)| \leqq v < 1$, $j, k = 1, \ldots, \mathrm{N}$. La preuve utilise une

transformation linéaire de l'inconnue u par une « pseudo transformation de Lorentz locale » qui gèle localement le mouvement des noyaux ainsi que la théorie abstraite des équations d'évolution.

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1. INTRODUCTION

We consider a time dependent Dirac equation

$$\partial_t u + i\mathrm{H}(t)u = 0, \qquad \mathrm{H}(t) = \alpha \cdot \mathrm{D} + (\varphi - \alpha \cdot \mathrm{A}) + m\beta u \tag{1.1}$$

where $\mathrm{D} = -i\partial_x = -i(\partial_1, \partial_2, \partial_3)$, $m \geqq 0$ and (A, φ) is the Liénard-Wiechert potential produced by a finite number of moving nuclei $q_k(t)$ with charges Z_k, $k = 1, \ldots, \mathrm{N}$:

$$(\mathrm{A}(t, x), \varphi(t, x)) = \sum_{k=1}^{\mathrm{N}} \left(\frac{\mathrm{Z}_k \dot{q}_k(s_k)}{|r_k| - r_k \cdot \dot{q}_k(s_k)}, \frac{\mathrm{Z}_k}{|r_k| - r_k \cdot \dot{q}_k(s_k)} \right), \tag{1.2}$$

$s_k = s_k(t, x)$ being the retarded time for the k-th nucleus:

$$t - s_k = |x - q_k(s_k)|,$$

and

$$r_k = x - q_k(s_k).$$

We assume that $\mathbb{R}^1 \ni t \to q_k(t) = (q_{k1}(t), \ldots, q_{k3}(t)) \in \mathbb{R}^3$ is of class C^3, $q_k(t) \neq q_j(t)$ for $k \neq j$ and

$$v = \sup\{|\dot{q}_k(t)| : -\infty < t < \infty, k = 1, \ldots, \mathrm{N}\} < 1, \tag{1.3}$$

$$\mathrm{Q} = \sup\{|\ddot{q}_k(t)| : -\infty < t < \infty, k = 1, \ldots, \mathrm{N}\} < \infty. \tag{1.4}$$

In what follows $\mathrm{H}^s = \mathrm{H}^s(\mathbb{R}^3, \mathbb{C}^4)$ is the standard Sobolev space of order $s \in \mathbb{R}^1$ and $\mathbb{H} = \mathrm{H}^0$. $\|u\|_s = \|(1 - \triangle)^{s/2} u\|$ is the standard norm in H^s and we write $\|\,.\,\|$ for $\|\,.\,\|_0$, where $\triangle$ is 3-dimensional Laplacian. For Banach spaces X and Y, $\mathrm{B}(\mathrm{X}, \mathrm{Y})$ is the set of bounded operators on X to Y, $\mathrm{B}(\mathrm{X}) = \mathrm{B}(\mathrm{X}, \mathrm{X})$ etc. C_* indicates the strong continuity of operator valued functions , e.g. $\mathrm{C}_*(\mathbb{R}^2, \mathrm{B}(\mathbb{H}))$ is the class of functions $\mathbb{R}^2 \to \mathrm{B}(\mathbb{H})$ which are strongly continuous.

The purpose of this paper is to solve (1.1) in an appropriate function space, by constructing the propagator $\mathrm{U}(t, s)$, $t, s \in \mathbb{R}^1$, which maps $u(s)$ to $u(t)$: $u(t) = \mathrm{U}(t, s)u(s)$ and prove the following theorem.

THEOREM. – *Let* $q_1(t), \ldots, q_N(t) \in C^3(\mathbb{R}^1, \mathbb{R}^3)$ *satisfy* (1.3), (1.4) *and* $q_j(t) \neq q_k(t)$ *for* $j \neq k$. *Suppose, in addition, that*

$$|Z_k| < \sqrt{3}/2, \; k=1, \ldots, N.$$

Then

$$H(\cdot) \in C_*(\mathbb{R}^1, B(H^1, \mathbb{H})) \cap C_*(\mathbb{R}^1, B(\mathbb{H}, H^{-1})).$$

There is a unique propagator $\{U(t, s), -\infty < t, s < \infty\}$ *with the following properties:*

(1) $U(\cdot, \cdot) \in C_*(\mathbb{R}^2, B(\mathbb{H})) \cap C_*(\mathbb{R}^2, B(H^1)) \cap C_*(\mathbb{R}^2, B(H^{-1}))$;

$$U(t, r)\, U(r, s) = U(t, s).$$

(2) $U(t, s) = U(s, t)^*$. *In particular*, $U(t, s) \in B(\mathbb{H})$ *is unitary in* $\mathbb{H}$.

(3) *For every* $f \in H^l$, $l=0, 1$, *we have*

$$i(\partial/\partial t)\, U(\cdot, s) f = H(\cdot)\, U(\cdot, s) f \in C(\mathbb{R}^1, H^{l-1}), \tag{1.5}$$

$$i(\partial/\partial s)\, U(t, \cdot) f = -U(t, \cdot)\, H(\cdot) f \in C(\mathbb{R}^1, H^{l-1}). \tag{1.6}$$

For proving the theorem, we want to apply to (1.1) a general theory of evolution equations such as given in [4]. In this attempt, we are faced with two major problems: one is the construction of the selfadjoint operator $H(t)$ for fixed $t \in \mathbb{R}^1$, and the other is the difficulty due to high singularity produced by moving Coulomb potentials, which makes it impossible to apply general results for evolution equations directly to (1.1).

The problems will be resolved by applying to (1.1) a "local pseudo-Lorentz transformation", a change of variables which resembles the spatial part of the boost by the velocity $\dot{q}_j(t)$ followed by the translation by $q_j(t)$, near $q_j(t)$ and which freezes the singularity of the potential at least for a small time interval $t \in I$; *cf.* Hunziker [3], where a local distortion technique is used to freeze the singularity of the potentials for solving time dependent Schrödinger equations with moving Coulomb singularities. If we introduce a new unknown function $\tilde{u}(t) = T(t)\, u(t)$, $t \in I$, using the family of unitary operators $T(t)$ associated with this transformation, the equation (1.1) converts into the form

$$\partial_t \tilde{u} + i \tilde{H}(t) \tilde{u} = 0,$$

$$\tilde{H}(t) = \Theta^{-1}(t)\, (H_0 + V + H'(t))\, \Theta^{-1}(t), \qquad t \in I, \tag{1.7}$$

where H_0, $H'(t)$, V and $\Theta(t)$ satisfy the following properties:

(*a*) H_0 is the free Dirac operator: $H_0 = \alpha \cdot D + m\beta$.

(*b*) V is a multiplication operator with a static Coulomb potential with N singularities: $V(x) = \sum_{k=1}^{N} Z_k |x - a_k|^{-1}$.

(*c*) $H'(t)$ is a family of formally selfadjoint differential operators of first order of the form $H'(t) = G(t, x).D + G'(t, x)$, where the components G_j,

$j=1, 2, 3$, of G and G′ are bounded 4×4 matrix valued functions such that $|\partial_t G(t, x)| \leqq C$, $|\partial_t G'(t, x)| \leqq C|x|^{-1}$ and $|G(t, x)| \leqq \varepsilon$ can be made arbitrarily small.

(*d*) $\Theta(t)$ is a multiplication operator with a Hermitian matrix valued smooth function $\Theta(t, x)$ such that $\Theta(t, x)^{\pm 1}$ is bounded with its derivatives.

It will be shown that the family of Dirac operators $H_0+V+H'(t)$, $t\in I$, is a smooth family of selfadjoint operators in $\mathbb{H}$ with constant domain H^1 with C_0^∞ as a common core. Hence, so is $\tilde{H}(t)$ and, this enables us to solve the modified equation (1.7) by applying the result in [4], which, in turn, gives the solution of (1.1) via the transformation $T(t)$.

The rest of the paper will be devoted to proving Theorem. In section 2, we shall examine the singularity of the potential $(A(t, x), \varphi(t, x))$. Then, in section 3, we introduce the local pseudo-Lorentz transformation. Using this transformation, we convert (1.1) into the form (1.7) and show that the modified Hamiltonian $\tilde{H}(t)$ satisfies the conditions (*a*) to (*d*) mentioned above. This will be done in section 4 and we shall complete the proof of Theorem in section 5. We shall denote various constants depending only on v and Q indiscriminately by C.

2. LIÉNARD-WIECHERT POTENTIALS

For solving (1.1), we need a precise information about the singularity of the potential $\varphi-\alpha\cdot A$. Since it is a sum of the Liénard-Wiechert potentials produced by a single moving nucleus, we treat here a single nucleus with charge Z. We let $x=q(t)$ represent the motion of the nucleus and assume $q\in C^l(\mathbb{R}, \mathbb{R}^3)$ $(l\geqq 2)$ with $|\dot{q}(t)|\leqq v<1$ and $|\ddot{q}(t)|\leqq Q<\infty$, $t\in\mathbb{R}^1$. We write $\Omega=\{(t, x): x\neq q(t)\}$.

LEMMA 2.1. – *The equation $t-s=|x-q(s)|$ uniquely determines the retarded time $s=s(t, x)\in C^l(\Omega)$ and $r(t, x)=x-q(s)\in C^l(\Omega)$. We have*

$$(1+v)^{-1}|x-q(t)| \leqq |r| \leqq (1-v)^{-1}|x-q(t)|. \tag{2.1}$$

Proof. – Since $\mathbb{R}^1\ni s\to s+|x-q(s)|\in\mathbb{R}^1$ is continuous and monotone increasing from $-\infty$ to ∞ by the assumption, $s=s(t, x)$ is uniquely determined as a continuous function. If $q(t)\neq x$, $|x-q(s)|\neq 0$ is C^l in (s, x) near $(s(t, x), x)$, and the implicit function theorem implies the smoothness property of s and r as stated in the lemma. Since

$$r=x-q(t)+(q(t)-q(s))$$

and

$$|q(t)-q(s)|\leqq v|t-s|=v|r|,$$

(2.1) follows immediately. ■

For a single moving nucleus we have, suppressing obvious variables, $\varphi-\alpha\cdot A=(1-\alpha\cdot\dot{q}(s))\varphi$ with $\varphi=Z(|r|-r\cdot\dot{q}(s))^{-1}$. Since the singularity of the potential appears only at the zero of

$$|r|-r.\dot{q}(s)\geqq(1-v)|r|\geqq(1-v)(1+v)^{-1}|x-q(t)|,$$

we write $y=x-q(t)$ and study the behavior of $|r|-r\cdot\dot{q}(s)$ as $|y|\to 0$. We denote by D/Dt the partial derivative with respect to t with y kept constant. We use the following two lemmas.

LEMMA 2.2. – *We have, with* $\rho=|r|-r\cdot\dot{q}(s)$,

$$Ds/Dt=1+\rho^{-1}r\cdot(\dot{q}(s)-\dot{q}(t)),\qquad \partial s/\partial y=-\rho^{-1}r. \tag{2.2}$$

Proof. – Differentiating $t-s=|r|$ and $r=x-q(s)=y+q(t)-q(s)$ by D/Dt, we have

$$1=\frac{Ds}{Dt}+\frac{D|r|}{Dt},\qquad \frac{D|r|}{Dt}=\frac{1}{|r|}r\cdot\frac{Dr}{Dt},\qquad \frac{Dr}{Dt}=\dot{q}(t)-\dot{q}(s)\frac{Ds}{Dt}.$$

Solving these equations yields the first identity of (2.2). The second can be proved similarly. ■

In what follows we write $f=\tilde{O}(|y|^k)$ $(k=1, 2, \ldots)$, if $|f|\leqq C|y|^k$ and $|Df/Dt|+|\partial f/\partial y|\leqq C|y|^{k-1}$, where C is a constant depending only on v and Q.

LEMMA 2.3. – *We have* $h_1\equiv q(s)-q(t)-(s-t)\dot{q}(t)=\tilde{O}(|y|^2)$ *and*

$$h_2\equiv y-(s-t)\dot{q}(t)=\tilde{O}(|y|).$$

Proof. – We prove the lemma for h_1 only. By Taylor's formula, we have

$$h_1=(s-t)^2\int_0^1(1-\theta)\ddot{q}(\theta s+(1-\theta)t)\,d\theta$$

and (2.1) implies $|h_1|\leqq Cy^2$. Using (2.2), we compute:

$$\begin{aligned}Dh_1/Dt&=(\dot{q}(s)-\dot{q}(t))Ds/Dt-(s-t)\ddot{q}(t)\\&=(s-t)\int_0^1(\ddot{q}(\theta s+(1-\theta)t)-\ddot{q}(t))\,d\theta\\&\qquad+\rho^{-1}(r\cdot(\dot{q}(s)-\dot{q}(t)))(\dot{q}(s)-\dot{q}(t)),\end{aligned}$$

and

$$\partial h_1/\partial y=-\rho^{-1}r\otimes(\dot{q}(s)-\dot{q}(t)).$$

Applying estimates (2.1), $|\rho^{-1}r|\leqq(1-v)^{-1}$ and

$$|\dot{q}(s)-\dot{q}(t)|\leqq Q(1-v)^{-1}|y|$$

to the identities above, we obtain

$$|Dh_1/Dt| + |\partial h_1/\partial y| \leqq C|y|,$$

and $h_1 = \tilde{O}(y^2)$. ■

Using $|r| = t-s$ and $r = y + (q(t) - q(s))$, we write, with the notation of Lemma 2.3,

$$|r| - r \cdot \dot{q}(s) = (1 - \dot{q}(t)^2)(t-s) - y \cdot \dot{q}(t) + h_1 \cdot \dot{q}(s) + h_2(\dot{q}(t) - \dot{q}(s)), \quad (2.3)$$

where, in virtue of Lemma 2.3, $h_1 \cdot \dot{q}(s) + h_2(\dot{q}(t) - \dot{q}(s)) = \tilde{O}(y^2)$. On the other hand, the square of the defining equation, $(t-s)^2 - r^2 = 0$, can be written in the form

$$\begin{aligned}(t-s)^2 - (h_2 - h_1)^2 &= (t-s)^2 - h_2^2 - h_1(h_1 - 2h_2)\\ &= (t-s)^2(1 - \dot{q}(t)^2) - 2(t-s)\dot{q}(t) \cdot y - y^2 - h_1(h_1 - 2h_2) = 0, \quad (2.4)\end{aligned}$$

where $h_1(h_1 - 2h_2) = \tilde{O}(|y|^3)$. Solving the last equation in (2.4) for $(t-s)$, we see

$$\begin{aligned}&(1 - \dot{q}(t)^2)(t-s) - y \cdot \dot{q}(t)\\ &\qquad = ((\dot{q}(t) \cdot y)^2 + (1 - \dot{q}(t)^2) y^2)^{1/2}(1 + \tilde{O}(|y|)), \quad (2.5)\end{aligned}$$

which with (2.3) implies the statements on φ in the following lemma.

LEMMA 2.4. – *Let* $q \in C^l(\mathbb{R}, \mathbb{R}^3)$, $(l \geqq 2)$ *with* $|\dot{q}(t)| \leqq v < 1$ *and* $|\ddot{q}(t)| \leqq Q < \infty$. *Set*

$$\varphi_0(t, x) = Z((\dot{q}(t) \cdot (x - q(t)))^2 + (1 - \dot{q}(t)^2)(x - q(t))^2)^{-1/2}.$$

Then we have

$$\varphi(t, x) = \varphi_0(t, x) + \varphi'(t, x) \quad (2.6)$$

and

$$\varphi(t, x) - A(t, x) \cdot \alpha = (1 - \alpha \cdot \dot{q}(t))\varphi_0(t, x) + \tilde{\varphi}(t, x), \quad (2.7)$$

where φ' *and* $\tilde{\varphi} \in C^{l-1}(\Omega)$ *respectively satisfy the estimates*

$$|\varphi'(t, x)| \leqq C, \ |\partial_t \varphi'| + |\partial_x \varphi'| \leqq C|x - q(t)|^{-1}, \quad (2.8)$$

$$|\tilde{\varphi}(t, x)| \leqq C, \ |\partial_t \tilde{\varphi}| + |\partial_x \tilde{\varphi}| \leqq C|x - q(t)|^{-1}. \quad (2.9)$$

Proof. – It suffices to show (2.7) and (2.9). We write

$$\begin{aligned}\varphi(t, x) - A(t, x) \cdot \alpha &= (1 - \alpha \cdot \dot{q}(s))\varphi(t, x)\\ &= (1 - \alpha \cdot \dot{q}(t))\varphi_0(t, x) + \alpha \cdot (\dot{q}(t) - \dot{q}(s))\varphi_0 + (1 - \alpha \cdot \dot{q}(s))\varphi'(t, x)\end{aligned}$$

and set $\tilde{\varphi}(t, x) = \alpha \cdot (\dot{q}(t) - \dot{q}(s))\varphi_0 + (1 - \alpha \cdot \dot{q}(s))\varphi'(t, x)$. Then (2.9) follows from (2.8), Lemma 2.1 and 2.2. ■

3. LOCAL PSEUDO-LORENTZ TRANSFORMATIONS

1. By a *symmetric cutoff function* we mean a real valued, nonnegative smooth function ζ on $\mathbb{R}^3$ such that $\zeta(x)=\Phi(|x|)$, with Φ having the following properties: $\Phi\in C^\infty(\mathbb{R})$, $\Phi(r)=0$ for $r\geqq\rho>0$, $\Phi(r)=1$ for $0\leqq r\leqq\rho'>0$, and strictly monotone decreasing in between. ρ (ρ') will be called the *outer* (*inner*) *radius* for ζ. The sup-norms of $|\partial\zeta(x)|$ and $|x||\partial\zeta(x)|$ will be called the *slope* and *characteristic number* of ζ, respectively.

LEMMA 3.1 (*cf.* Hopf [2, p. 13]). – *There is a symmetric cutoff function with a given outer radius* ρ *and with arbitrarily small characteristic number.*

Proof. – Let $0\leqq\Psi_n\in C_0^\infty(\mathbb{R})$, $n=1, 2, \ldots$, with supports in $(0, \rho)$ and with $\Psi_n(r)\uparrow 1$, $n\to\infty$, for $r\in(0, \rho)$. Set

$$\Phi_n(r)=\lambda_n^{-1}\int_r^\infty s^{-1}\Psi_n(s)\,ds,\qquad \lambda_n=\int_0^\infty s^{-1}\Psi_n(s)\,ds.$$

Then $\zeta_n(x)=\Phi_n(|x|)$ is a symmetric cutoff function with outer radius ρ. Since $\lambda_n\to\infty$ by monotone convergence theorem, we have $\sup|r\Phi_n'(r)|\to 0$ as $n\to\infty$. ■

Remark. – (*a*) A small characteristic number γ requires a small inner radius ρ' and a large slope. Indeed, it is easy to see that $\rho'/\rho\leqq e^{-1/\gamma}$ and $\sup|\partial\zeta|\geqq e^{1/2\gamma}/2\rho$.

(*b*) A simple example of a symmetric cutoff function is given via $\Phi(r)=\Xi(\log(1+\rho/\varepsilon r)/\log(1+1/\varepsilon))$, where $\Xi\in C^\infty(\mathbb{R})$ is an increasing function such that $\Xi(s)=0$ for $s\leqq 1$, $\Xi(s)=1$ for $s\geqq 2$ and $0<\Xi(s)<1$ in between. The characteristic number of this function is $O(1/\log(1/\varepsilon))$.

2. Let $q=(q_1, q_2, q_3)\in C^l(\mathbb{R}, \mathbb{R}^3)$ ($l\geqq 2$) with $q(0)=0$ and $|\dot q(t)|<1$. (In this section q_j, $j=1, 2, 3$, denotes the j-th component of q. This should not be confused with the notation in other sections where q_k represents the k-th nucleus.) Using a symmetric cutoff function ζ, we define a transformation $x\to\tilde x=L_{q,\zeta}(x, t)$ by

$$\begin{aligned}\tilde x&=x-\zeta(x)q(t)\\&\quad+((1-\zeta(x)^2\dot q(t)^2)^{-1/2}-1)\dot q(t)^{-2}((x-\zeta(x)q(t))\cdot\dot q(t))\dot q(t).\end{aligned}\tag{3.1}$$

This is a C^∞-map of $\mathbb{R}^3$ into itself for fixed $t\in\mathbb{R}$, and depends on t in C^{l-1}-manner; the possibility that $\dot q(t)=0$ for some t does not cause any difficulty, since the dependence of (3.1) on $\dot q(t)$ is analytic for $|\dot q(t)|<1$.

If we take the coordinate system in which $q(t)$ is parallel to the x_1-axis (which may depend on t), (3.1) takes the form

$$\left.\begin{aligned}&\tilde x_1=(1-\zeta(x)^2\dot q(t)^2)^{-1/2}(x_1-\zeta(x)q_1(t)),\\&\tilde x_2=x_2-\zeta(x)q_2(t),\qquad \tilde x_3=x_3-\zeta(x)q_3(t).\end{aligned}\right\}\tag{3.1 a}$$

Let ρ and ρ' denote the outer and inner radii of ζ. Then (3.1) reduces to $\tilde{x}=x$ for $|x|\geqq\rho$ where $\zeta(x)=0$. Thus (3.1) fixes all points outside the ball $B_\rho=\{x:|x|\leqq\rho\}\subset\mathbb{R}^3$. For $|x|\leqq\rho'$, on the other hand, $\zeta(x)=1$ and (3.1 *a*) looks like the spatial part of the Lorentz transformation. As will be seen below, it has the merit of converting the Liénard-Wiechert potential into a static Coulomb potential.

To study the behavior of the transformation in more detail, we shall compute the Jacobian matrix. To simplify the notation, we set

$$\omega(x,t)=(1-\zeta(x)^2\dot{q}(t)^2)^{-1/2},\qquad 1\leqq\omega\leqq\omega_0\equiv(1-\dot{q}(t)^2)^{-1/2}. \tag{3.2}$$

A straightforward computation then gives (for simplicity we suppress the arguments in ζ, q, $\dot{q}$ and ω)

$$\begin{aligned}\partial\tilde{x}=id-\partial\zeta\otimes q+(\omega-1)\dot{q}^{-2}\dot{q}\otimes q\\ -(\omega^3-1)\dot{q}^{-2}(q\cdot\dot{q})\,\partial\zeta\otimes\dot{q}+\omega^3(x\cdot\dot{q})\,\zeta\,\partial\zeta\otimes\dot{q}.\end{aligned} \tag{3.3}$$

In the special coordinate system considered above, this simplifies to

$$\left.\begin{aligned}\partial_j\tilde{x}_1=\omega\delta_{j1}+\omega^3(\zeta\,\partial_j\zeta\,\dot{q}^2x_1-\partial_j\zeta\,q_1),\qquad \partial_j\tilde{x}_k=\delta_{jk}-\partial_j\zeta\,q_k,\\ j=1,2,3,\qquad k=2,3.\end{aligned}\right\} \tag{3.3 a}$$

(3.3 *a*) shows that the main part of the Jacobian is a diagonal matrix with element $(\omega, 1, 1)$, where $\omega\geqq 1$, and the remaining elements are majorized by $\omega^3(\gamma+M|t|)$, where $\omega^3\leqq(1-\dot{q}^2)^{-3/2}$ and γ and M denote the characteristic number and the slope of ζ, respectively. (Note that $|q(t)|\leqq|t|$ because $q(0)=0$ and $|\dot{q}|<1$.) Since we can take γ arbitrarily small for a given ρ (Lemma 3.1), this leads to

LEMMA 3.2. — *Let* $q\in C^l(\mathbb{R},\mathbb{R}^3)$ $(l\geqq 2)$ *with* $q(0)=0$, $|\dot{q}(t)|<1$. *Given any* $\rho>0$, *we can choose a symmetric cutoff function* ζ *with outer radius* ρ, *and a number* $\tau>0$ *in such a way that the following conditions are met.*

(1) (3.1) *is a* C^∞*-diffeomorphism of* $\mathbb{R}^3$ *onto itself for* $|t|\leqq\tau$, *with the Jacobian determinant* $J>1/2$, *say, and depends on t in* C^{l-1}*-manner.*

(2) *For each* $t\in[-\tau,\tau]$, *the ball* B_ρ *is mapped onto itself, while each point outside it is fixed. Moreover,* $|q(t)|<\rho'$, *where* ρ' *is the inner radius of* ζ.

For later use we deduce an estimate for $\partial_t\tilde{x}$, which depends on t in C^{l-2}-manner:

$$\partial_t\tilde{x}=-\omega\zeta\dot{q}+O(\rho)+O(t); \tag{3.3 b}$$

here the first term comes from differentiating ζq, which appears twice in (3.1), while the remaining terms contain either a factor $x\zeta(x)=O(\rho)$ or $q(t)=O(t)$, with other factors uniformly bounded.

4. THE MODIFIED DIRAC OPERATOR

We now consider the Dirac equation

$$\partial_t u + i\mathrm{H}(t)u=0, \qquad \mathrm{H}(t)=\alpha\cdot \mathrm{D}+(\varphi-\mathrm{A}\cdot\alpha)+m\beta \tag{1.1}$$

We wish to convert the equation (1.1) into a more tractable form. To explain the basic idea, we first consider the case when (A, φ) is the Liénard-Wiechert potential due to a single moving nucleus with charge Z. As in section 2, we let $x=q(t)$ represent the motion of the nucleus, where $q\in \mathrm{C}^3(\mathbb{R}, \mathbb{R}^3)$, with $q(0)=0$, $|\dot{q}(t)|\leqq v<1$ and $|\ddot{q}(t)|\leqq \mathrm{Q}<\infty$. It was shown in Lemma 2.4 that

$$\varphi-\mathrm{A}\cdot\alpha=(1-\alpha\cdot\dot{q}(t))\,\varphi_0+\tilde{\varphi}, \tag{4.1}$$

$$\varphi_0=\mathrm{Z}\{((x-q(t))\cdot\dot{q}(t))^2+(1-|\dot{q}(t)|^2)\,|x-q(t)|^2\}^{-1/2}, \tag{4.1 a}$$

where $\tilde{\varphi}\in \mathrm{C}^2(\Omega)$ is a Hermitian matrix-valued function which satisfies (2.9).

We want to freeze the motion of the nucleus. To this end we apply to (1.1) a local pseudo-Lorentz transformation $(t, \tilde{x})=\mathrm{L}_{q,\zeta}(t, x)$ given by Lemma 3.2, restricting t within $(-\tau, \tau)$ in the sequel; actually we shall later have to restrict to a smaller interval. Since we want preserve the formal selfadjointness of the Hamiltonian in (1.1), we introduce a unitary transformation $\mathrm{T}(t)$ from $\mathbb{H}=\mathrm{L}^2(\mathbb{R}^3, dx)$ to $\tilde{\mathbb{H}}=\mathrm{L}^2(\mathbb{R}^3, d\tilde{x})$ by

$$\mathrm{T}(t)\,u(\tilde{x})=\mathrm{J}(t, x)^{-1/2}\,u(x), \tag{4.2}$$

and transform the unknown function by

$$\tilde{u}(t, \tilde{x})=\mathrm{T}(t)\,u(t, \cdot)\,(\tilde{x})=\mathrm{J}(t, x)^{-1/2}\,u(t, x) \tag{4.2 a}$$

where J is the Jacobian determinant for $\mathrm{L}_{q,\zeta}$ (*see* Lemma 3.2). Note that $\mathrm{T}(t)$ is not only a smooth family of unitary operators but also of isomorphisms of H^s for every $s\in\mathbb{R}$.

A straightforward substitution using (3.3) leads to the following modified equation, where the arguments in $\zeta(x)$, $q(t)$, etc. are suppressed for simplicity, $\omega=(1-\zeta^2\dot{q}^2)^{-1/2}$ and $\tilde{\mathrm{D}}=-i\partial_{\tilde{x}}$.

$$\partial_t\tilde{u}+i\tilde{\mathrm{H}}(t)\,\tilde{u}=0, \qquad \tilde{\mathrm{H}}(t)=\tilde{\mathrm{H}}_0(t)+\tilde{\mathrm{H}}'(t), \tag{4.3}$$

$$\tilde{\mathrm{H}}_0(t)=\{\alpha-\omega\zeta\dot{q}+(\omega-1)\,\dot{q}^2(\alpha\cdot\dot{q})\,\dot{q})\}\cdot\tilde{\mathrm{D}}+(1-\zeta\alpha\cdot\dot{q})\,\varphi_\zeta+m\beta, \tag{4.3 a}$$

$$\tilde{\mathrm{H}}'(t)=\mathrm{F}\cdot\tilde{\mathrm{D}}+\mathrm{W}+\tilde{\varphi}+(\zeta-1)\,\alpha\cdot\dot{q}\,\varphi_\zeta. \tag{4.3 b}$$

Here we have replaced φ_0 with φ_ζ, which is obtained from (4.1 *a*) by replacing q by ζq, the difference being included in the term W; note that the difference is a bounded function because $\zeta=1$ for $|x|\leqq\rho'$, where ρ' is the inner radius of ζ (recall that by Lemma 3.2, (2), τ has been chosen so small that the singularity q of φ_0 is inside the ball $\mathrm{B}_{\rho'}$); W also includes $\mathrm{J}^{-1}(\partial_t\mathrm{J}-\alpha\cdot\partial_x\mathrm{J})$, which is also bounded (note that $\partial_t\mathrm{J}$ and $\partial_x\mathrm{J}$ involve the second derivatives of ζ, but these are bounded functions); F is a matrix-valued 3-vector, including the expression $O(\rho)+O(t)$ in (3.3 b), as well as the term derived from the second line in (3.3), which are of the order $O(\gamma)+O(\mathrm{M}\,t)$, as was shown in the proof of Lemma 3.2. (Here ρ is the outer radius and γ is the characteristic number, and M is the slope of ζ.) Thus $|\mathrm{F}|$ can be made arbitrarily small by first choosing ρ and γ small (which is possible by Lemma 3.1), and then reducing τ further if necessary. Note that the derivatives in x of F, W, $\partial_t \mathrm{F}$ and $\partial_t \mathrm{W}$ are also bounded because q is C^3 and that $|\partial_t \tilde{\varphi}| \leqq \mathrm{C}|\tilde{x}|^{-1}$. Hence,

$$\tilde{\mathrm{H}}'(\cdot) \in \mathrm{C}^1_*((-\tau, \tau), \mathrm{B}(\mathrm{H}^1, \tilde{\mathbb{H}})) \cap \mathrm{C}^1_*((-\tau, \tau), \mathrm{B}(\tilde{\mathbb{H}}, \mathrm{H}^{-1})).$$

In (4.3 a-3 b), the space variables are $\tilde{x}$ rather than x, so that ζ and φ should be regarded as functions of t and $\tilde{x}$. Then $\tilde{\mathrm{H}}(t)$ is formally selfadjoint for each t, as is guaranteed by its derivation. Hence it is a symmetric operator in $\tilde{\mathbb{H}} = \mathrm{L}^2(\mathbb{R}^3, d\tilde{x})$.

According to Lemma 3.2, $|x| \leqq \rho$ is equivalent to $|\tilde{x}| \leqq \rho$ so that $\zeta = 0$ if $|\tilde{x}| \geqq \rho$. Moreover, F and W vanish identically there. In the exterior of B_ρ, therefore, the operator $\tilde{\mathrm{H}}(t)$ is the standard Dirac operator $\alpha \cdot \tilde{\mathrm{D}} + (1 - \alpha \cdot \dot{q})\varphi + m\beta$, where the potential φ is bounded.

Now φ_ζ takes a simple form:

$$\varphi_\zeta = \mathrm{Z}\,\omega\,|\tilde{x}|^{-1}. \tag{4.4}$$

To see this, we may assume that $\dot{q} \neq 0$ (otherwise it is obvious). Let $y = x - \zeta q$ and let $y = y' + y''$ be its decomposition into parallel and perpendicular components to $\dot{q}$. Then (3.1) shows that

$$\tilde{x} = y + (\omega - 1)\,y' = y'' + \omega\,y',$$

hence

$$\tilde{x}^2 = y''^2 + \omega^2 y'^2 = y^2 + (\omega^2 - 1)\,y'^2 = \omega^2\,((1 - \zeta^2 \dot{q}^2)\,y^2 + \zeta^2 \dot{q}^2 y'^2),$$

which proves (4.4).

Also the first order part of $\mathrm{H}_0(t)$ can be reduced to a simple form. To see this we define a quantity θ by

$$\theta = \theta(t, x) = \frac{1}{2|\dot{q}|} \log\left(\frac{1+\zeta|\dot{q}|}{1-\zeta|\dot{q}|}\right) = \zeta\,(1 + \zeta^2 \dot{q}^2/3 + \zeta^4 \dot{q}^4/5 + \ldots), \tag{4.5}$$

which is analytic in $\dot{q}$ for $|\dot{q}| < 1$. The following relation can be verified easily:

$$\cosh(\theta|\dot{q}|) = \omega, \qquad \sinh(\theta|\dot{q}|) = \omega\zeta|\dot{q}|, \tag{4.6 a}$$

$$e^{-\theta\alpha\cdot\dot{q}} = \omega\,(1 - \zeta\,\alpha\cdot\dot{q}),\ (\alpha\cdot\dot{q})\,e^{-\theta\alpha\cdot\dot{q}} = \omega\,(\alpha - \zeta\dot{q})\cdot\dot{q}, \tag{4.6 b}$$

$$|e^{k\,\theta\alpha\cdot\dot{q}}| \leqq ((1 + |\dot{q}|)/(1 - |\dot{q}|))^{|k|}, \qquad k \in \mathbb{R}. \tag{4.6 c}$$

LEMMA 4.1. — *Set* $\Theta = e^{\theta\alpha\cdot\dot{q}/2}$. *Then* $\Theta^{\pm 1}$ *is a smooth family of bounded selfadjoint operators in* $\mathbb{H}$ *which are also isomorphisms of* H^s, $s \in \mathbb{R}$. *We* *have*

$$\Theta\{\alpha-\omega\zeta\dot{q}+(\omega-1)\dot{q}^2\alpha\cdot\dot{q})\dot{q}\}\Theta=\alpha, \tag{4.7 a}$$

$$\Theta(1-\zeta\alpha\cdot\dot{q})\varphi_\zeta\Theta=Z|\tilde{x}|^{-1}, \qquad \Theta\beta\Theta=\beta. \tag{4.7 b}$$

Note that $\Theta=1$ for $|\tilde{x}|\geqq\rho$ (because $\theta=0$ there).

Proof. – (4.7 *a*) is obvious if $\dot{q}=0$, so we may assume $\dot{q}\neq 0$. We decompose the vector α into $\alpha=\alpha'+\alpha''$, where $\alpha'=\dot{q}^{-2}(\alpha\cdot\dot{q})\dot{q}$ is the component parallel to $\dot{q}$ and $\alpha''=\alpha-\alpha'$ is the perpendicular. Then we have

$$\alpha-\omega\zeta\dot{q}+(\omega-1)\dot{q}^{-2}(\alpha\cdot\dot{q})\dot{q}=\omega(\alpha'-\zeta\dot{q})+\alpha''=e^{-\theta\alpha\cdot\dot{q}}\alpha'+\alpha'', \tag{4.8}$$

where we have used the relation

$$e^{-\theta\alpha\cdot\dot{q}}\alpha'=\omega(1-\zeta\alpha\cdot\dot{q})\alpha'=\omega(\alpha'-\zeta(\alpha\cdot\dot{q})\dot{q}^{-2}(\alpha\cdot\dot{q})\dot{q})=\omega(\alpha'-\zeta\dot{q}).$$

If we multiply (4.8) from both sides with $\Theta=e^{\theta\alpha\cdot\dot{q}/2}$, where $\alpha\cdot\dot{q}$ commutes with α' and anti-commutes with α'', the result is $\alpha'+\alpha''=\alpha$, yielding (4.7 *a*).

The first part of (4.7 *b*) follows from (4.4) and (4.6 *b*). The second one is true since $\alpha\cdot\dot{q}$ and β anticommute.

In this way we arrive at the form

$$\Theta\tilde{H}_0(t)\Theta=\alpha\cdot\tilde{D}+m\beta+Z|\tilde{x}|^{-1}+W'', \tag{4.9}$$

where W'' is a matrix valued function arising by commuting Θ and $\tilde{D}$, and is bounded with its derivatives up to second order in t and x. Except for this bounded perturbation, (4.9) is the Dirac operator with the static potential $Z|\tilde{x}|^{-1}$.

Next we consider the case of N moving nuclei. Let $x=q_j(t)$, $j=1, \ldots, N$, be their orbits. The potential is given by $\varphi=\sum_{j=1}^{N}\varphi_j$, $A=\sum_{j=1}^{N}A_j$, with obvious notation.

We introduce local distortion near $a_j=q_j(0)$ for each j. To this end we choose $\rho>0$ sufficiently small that N balls $B_j=\{x:|x-a_j|\leqq\rho\}$ are disjoint, and a symmetric cutoff function ζ with outer radius ρ. Then we define local pseudo-Lorentz transformation

$$L_j(t, x)=a_j+L_{q_j-a_j,\zeta}(t, x-a_j).$$

We shall choose ζ in such a way that the preceding results for a single-nucleus system hold true for each nucleus, with sufficiently small τ. Then the N transformations merge into a single diffeomorphism $(t, x)\to(t, \tilde{x})=L(t, x)$ of the slab S_τ, with the Jacobian determinant bounded and bounded away from zero, which fixes each point outside $\bigcup_{j=1}^{N}B_j$.

If we set $\tilde{u}(t, \tilde{x}) = \mathrm{T}(t) u(t, \cdot)(\tilde{x}) = \mathrm{J}^{-1/2} u(t, x)$ as in (4.2 *a*), (1.1) is transformed into (4.3), where $\tilde{\mathrm{H}}(t)$ takes different forms in different parts of S_τ. Let Θ_j be the operator corresponding to the Θ used above. Since $\Theta_j = \mathrm{id}$ outside B_j, $\Theta_1, \ldots, \Theta_\mathrm{N}$ combine smoothly into a single operator Θ, so that we have a generalization of (4.9):

$$\Theta \tilde{\mathrm{H}}_0(t) \Theta = \alpha \cdot \tilde{\mathrm{D}} + m\beta + \sum_{j=1}^{\mathrm{N}} \mathrm{Z}_j |\tilde{x} - a_j|^{-1} + \mathrm{W}', \tag{4.10}$$

where W′ is a bounded function with its derivatives in (t, x) up to second order, while $\tilde{\mathrm{H}}'(\cdot) \in \mathrm{C}^1_*((-\tau, \tau), \mathrm{B}(\mathrm{H}^1, \tilde{\mathbb{H}})) \cap \mathrm{C}^1_*((-\tau, \tau), \mathrm{B}(\tilde{\mathbb{H}}, \mathrm{H}^{-1}))$ has a form analogous to (4.3 *b*). Here the condition $q_k \in \mathrm{C}^3$, $k = 1, \ldots, \mathrm{N}$ is used for showing the C^1-property of $\tilde{\mathrm{H}}'(t)$.

LEMMA 4.2. – *If* $|\mathrm{Z}_j| < \sqrt{3}/2$, $\tilde{\mathrm{H}}_0(t)$ *is selfadjoint with domain* H^1. *Moreover we have,*

$$\|\tilde{\mathrm{H}}_0(t) f\|^2 \geqq \mathrm{C}\|f\|_1^2 - \mathrm{M}\|f\|^2, \qquad f \in \mathrm{H}^1, \tag{4.11}$$

where $\mathrm{C} > 0$ *depends only on* v.

Proof. – $\Theta \tilde{\mathrm{H}}_0(t) \Theta$ is, except for a bounded perturbation, identical with the Dirac operator with N static Coulomb singularities with charges Z_j smaller than $\sqrt{3}/2$. Therefore it is selfadjoint. Indeed this is known for a single nucleus (*cf.* Arai-Yamada [1] and Schmincke [5]); for many nuclei, it can be proved by a standard method using a partition of unity to isolate the singularities. The desired result follows from this, since $\Theta^{\pm 1}$ are matrix valued functions with norm not exceeding a number depending only on $|\dot{q}_j|$, $j = 1, \ldots, \mathrm{N}$.

THEOREM 4.3. – *If* $|\mathrm{Z}_j| < \sqrt{3}/2$, $\tilde{\mathrm{H}}(t)$ *is selfadjoint and depends smoothly on t. More precisely, we can choose* ζ *and* τ *in such a way that for* $t \in (-\tau, \tau)$, $\tilde{\mathrm{H}}(t)$ *is selfadjoint in* $\mathbb{H}$ *with constant domain* H^1 *and* $\tilde{\mathrm{H}}(\cdot) \in \mathrm{C}^1_*((-\tau, \tau), \mathrm{B}(\mathrm{H}^1, \tilde{\mathbb{H}})) \cap \mathrm{C}^1_*((-\tau, \tau), \mathrm{B}(\tilde{\mathbb{H}}, \mathrm{H}^{-1}))$.

Proof. – According to Lemma 4.2, it suffices to show that $\tilde{\mathrm{H}}'(t)$ is bounded relative to $\tilde{\mathrm{H}}_0(t)$ with small relative bound. This is true since, as is remarked above, F can be made arbitrarily small by choosing γ and τ small; here it is essential that making γ small may affect ζ but not the constant C in (4.11). ■

5. PROOF OF THEOREM

We are ready to prove Theorem by applying the abstract theory of evolution equations given in [4].

Proof of Theorem. – In virtue of the standard continuation argument, it suffices to prove the theorem in a small interval $\mathrm{I} = (-\tau, \tau)$. Theorem

4.3 shows that $\tilde{\mathrm{H}}(t)$ in the modified equation (4.3) is selfadjoint in $\mathbb{H}$ with constant domain H^1 and $\tilde{\mathrm{H}}(\cdot)\in \mathrm{C}^1_*(\mathbb{R}^1, \mathrm{B}(\mathrm{H}^1, \tilde{\mathbb{H}}))$. Hence, due to a result in [4], there is a unique propagator $\{\tilde{\mathrm{U}}(t, s): -\tau<t, s<\tau\}$ for the family $\tilde{\mathrm{H}}(t)$ that satisfies the statements of Theorem with $\tilde{\mathrm{H}}(t)$ and $\tilde{\mathrm{U}}(t, s)$ replacing $\mathrm{H}(t)$ and $\mathrm{U}(t, s)$, respectively. Define using the transformation $\mathrm{T}(t)$ of (4.2) (or its generalization to N-nuclei case), $\mathrm{U}(t, s)=\mathrm{T}(t)^{-1}\tilde{\mathrm{U}}(t, s)\mathrm{T}(s)$. Since $\mathrm{T}(t)$ is a smooth family of unitary operators from $\mathbb{H}$ to $\tilde{\mathbb{H}}$ which are also isomorphisms of $\mathrm{H}^{\pm 1}$, it is easy to see that $\mathrm{U}(t, s)$ satisfies the statement of Theorem for $t, s\in(-\tau, \tau)$. To prove the uniqueness of the propagator $\mathrm{U}(t, s)$, it suffices to show that $\tilde{\mathrm{U}}(t, s)=\mathrm{T}(t)\mathrm{U}(t, s)\mathrm{T}(s)^{-1}$ is a propagator associated with the family $\{\tilde{\mathrm{H}}(\cdot)\}$. This, however, is obvious from the derivation. ■

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