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Time Boundedness of the Energy for the Charge Transfer Model

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Abstract. The energy behavior of the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\psi=\frac{-1}{2m}\Delta\psi+\sum_{j=1}^{N}V_j(x-y_j(t))\psi$$

is discussed, where the $y_j(t)$ are trajectories of classical scattering. In particular, we prove that the energy cannot become arbitrarily large as $t\to\infty$.

1. Introduction and Results

The charge transfer model describes a system of one quantum particle, e.g., an electron, and N others, which can be treated classically because they have a much greater mass (see [1–5, 8–10]). We suppose that the trajectories $y_j(t), j=1,\ldots,N$, of the heavy particles are given and cause a time-dependent potential for the first one. So we have to consider the Schrödinger equation

$$\frac{d}{dt}\psi(t)=-iH(t)\psi(t) \tag{1.1}$$

in the Hilbert space $L^2(\mathbb{R}^\nu)$, where $H(t)=H_0+V(t)$, $H_0=-\frac{1}{2m}\Delta$ and

$$V(t)=\sum_{j=1}^{N}V_j(x-y_j(t)).$$

In addition to the self-adjointness of all $H(t)$, $t\in\mathbb{R}$, one needs some smoothness of $V(t)$ for the existence of the time evolution. If the $y_j(t)$ are continuously differentiable and the $\nabla V_j(x)$ are H_0-bounded, then the existence is well known (Theorem X.71 in [7]). This does not include the Coulomb potential $V_j(x)=|x|^{-1}$ for dimension $\nu=3$, which is the most important in the charge transfer model. However, some recent papers ([5, 8, 11]) show that there also exists a time evolution for potentials $V_j(x)$ with singularities like $|x|^{-\frac{3}{2}+\varepsilon}$, $\varepsilon>0$, $\nu=3$.

Because of the explicit time dependence of the Hamiltonian, we have a loss of energy conservation. So we can ask, which energy behavior can occur? Are there some initial states with an energy expectation which goes to infinity for large times? We will show that this cannot happen for $y_j(t)$ arising from classical scattering in the sense of assumption (1) (see below). The energy boundedness [in the weaker sense of Corollary 4.2(b)] is necessary for asymptotic completeness. Furthermore, we will see in Sect. 2 that for large times the energy decreases if the electron moves repeatedly from one center of force to another. This feature is important in the proof of asymptotic completeness [9], too.

We will assume the following:

1. The paths $y_j(t), j=1, \ldots, N$, are twice continuously differentiable with

$$\ddot{y}_j(t) = \frac{d^2}{dt^2} y_j(t) \in L^1(\mathbb{R}_+, dt). \tag{1.2}$$

There are α, $t_1 > 0$ such that

$$|y_j(t) - y_l(t)| \geqq \alpha t \quad \text{for} \quad t \geqq t_1, j \neq l. \tag{1.3}$$

2. Every V_j is an H_0-bounded multiplication operator with relative bound zero.
3. The time evolution exists; i.e., there is a family of unitary operators $\{U(t,s)\}_{t,s\in\mathbb{R}}$ such that
   (a) $U(t,t) = \mathbb{1}$ for all $t \in \mathbb{R}$;
   (b) $U(t,s)U(s,r) = U(t,r)$ for all $t, s, r \in \mathbb{R}$;
   (c) $U(t,s)D(H_0) = D(H_0)$ and $\psi(t) \equiv U(t,s)\psi$ is continuously differentiable with respect to t, satisfying (1.1) for each $\psi \in D(H_0)$ and $s \in \mathbb{R}$.
4. Outside a compact set K_j every potential $V_j(x)$ has a derivative in $L^\infty(\mathbb{R}^\nu \setminus K_j)$ such that for some $R > 0$,

$$\|\nabla V_j(x) F(|x| > r)\| \in L^1([R, \infty), dr), \tag{1.4}$$

where the orthogonal projector $F(|x| > r)$ is given by multiplication with the characteristic function of the indicated region.

Of course, classical trajectories $y_j(t)$, which are outgoing in the sense of (1.3), satisfy (1.2) if the forces between the heavy particles are decaying like the forces acting on the light particle [see (1.4)].

By a Cauchy argument, it follows that

$$v_j := \lim_{t \to \infty} \dot{y}_j(t)$$

exists with $v_j \neq v_l$ for $j \neq l$. With the second assumption and the Kato-Rellich theorem, $H(t)$ is self-adjoint on $D(H(t)) = D(H_0)$. Furthermore, we get a uniform lower bound for the Hamiltonian, i.e., for some $M > 0$ and all $t \in \mathbb{R}$ we have

$$H(t) + M \geqq 0. \tag{1.5}$$

Now we state our main result.

Theorem 1.1. *Suppose the assumptions* (1)–(4) *are satisfied. Then for each initial time* $s \in \mathbb{R}$ *and each* $\psi \in D(H_0)$, *the time evolution* $\psi(t) = U(t,s)\psi$ *has a uniformly* *bounded energy expectation*, i.e.,

$$\sup_{t \geqq s} (\psi(t), H(t)\psi(t)) < \infty \tag{1.6}$$

and

$$\sup_{t \geqq s} (\psi(t), H_0\psi(t)) < \infty . \tag{1.7}$$

The operator boundedness with bound zero in assumption (2) implies form boundedness with bound zero. Hence, (1.6) and (1.7) are equivalent. The proof of (1.7) is given in the next two sections. In the following we show that an appropriate energy expression has a controllable time derivative. For the definition of this expression we need some vectors and some functions of time satisfying (2.1)–(2.4). The existence of these are given in Sect. 3.

Theorem 1.1 is an extension of the first part of [9], where the energy boundedness is an essential tool for the proof of asymptotic completeness. Independently of this work, Graf [2] has also proved that the energy cannot increase without bound. Although he has used a different method, the assumptions are essentially the same.

2. Change of the Energy

Since $H(t)\psi(t)$ is continuous in t (Assumption 3.c), we get that $\sup_{s \leqq t \leqq t_0} (\psi(t), H(t)\psi(t))$ is bounded for every fixed $t_0 \geqq s$. Unfortunately we are not able to show that the time derivative of the energy expectation is in $L^1([t_0, \infty), dt)$ for some t_0,

$$\frac{d}{dt}(\psi(t), H(t)\psi(t)) = - \sum_{j=1}^{N} \dot{y}_j(t) \cdot (\psi(t), \nabla V_j(x - y_j(t))\psi(t)) .$$

So we try to find an energy expression whose derivative can be estimated.

For $N=1$ and $y_1(t) \equiv tv_1$, we could change to the rest frame of the center of force by a Galilei transformation. There we have energy conservation. Equivalently we could consider:

$$\tilde{H}(t) = \frac{1}{2m}(P - mv_1)^2 + V_1(x - y_1(t)) = H(t) - v_1 \cdot P + \frac{m}{2} v_1^2$$

in the original frame. Here $P := -i\nabla$ denotes the momentum operator.

While $\frac{m}{2} v_1^2$ is only an unimportant constant, the time derivative of $v_1 \cdot P$, i.e., the commutator $i[H(t), v_1 \cdot P]$, cancels the uncontrollable derivative of the potential. Thus the expectation of $\tilde{H}(t)$ is constant.

In the general situation we take instead of $v_1 \cdot P$ an operator $A(t)$. In a neighborhood of each $y_j(t)$, this operator $A(t)$ should be $\dot{y}_j(t) \cdot P$ (plus a real bounded function of t). These neighborhoods should grow linearly in time.

Since our intuition is based on $y_j(t)$ which are straight lines, we need the following

Lemma 2.1. $y_j(t) = tv_j + o(t)$ *for* $t \to \infty$.

Proof. Let $\varepsilon>0$. Take $t_0>0$ such that $\sup_{t\geqq t_0}|\dot{y}_j(t)-v_j|<\frac{\varepsilon}{2}$. Then

$$\begin{aligned}\frac{1}{t}|y_j(t)-tv_j| &\leqq \frac{1}{t}\left|y_j(0)+\int_0^{t_0}(\dot{y}_j(s)-v_j)ds\right|+\frac{1}{t}\int_{t_0}^{t}|\dot{y}_j(s)-v_j|ds\\ &\leqq \frac{1}{t}\,\mathrm{const}_{t_0}+\frac{\varepsilon}{2}\\ &<\varepsilon \text{ for } t\geqq t_1>t_0 \text{ and } t_1 \text{ large}. \quad \square\end{aligned}$$

Assume that there are finitely many $w_k\in\mathbb{R}^\nu$ and real $\lambda_k(t)$, $k=1,\dots,M$, satisfying

$$w_k\cdot v_j\neq w_k^2 \quad \text{for all } j,k, \tag{2.1}$$

$$\sum_{\substack{k\\ w_k\cdot v_j>w_k^2}}\lambda_k(t)w_k=\dot{y}_j(t) \quad \text{for all } j, \tag{2.2}$$

$$\dot{\lambda}_k(t)\in L^1(\mathbb{R}_+,dt), \tag{2.3}$$

and

$$\lim_{t\to\infty}\lambda_k(t)>0. \tag{2.4}$$

In the case $\dot{y}_j(t)\equiv v_j$, the $\lambda_k(t)$ can be chosen independent of t. The existence is shown in Sect. 3. Now we define the energy expression which we mentioned before:

$$B(t)=H(t)-A(t), \tag{2.5}$$

where

$$A(t)=\sum_{k=1}^{M}\lambda_k(t)w_k\cdot\{f_kP^{(k)}+P^{(k)}f_k\}, \tag{2.6}$$

$$P^{(k)}=P-mw_k, \tag{2.7}$$

$$f_k=f_k(t,x)=\varphi\left(\frac{1}{t^\alpha}w_k\cdot[x-tw_k]\right), \tag{2.8}$$

$$\tfrac{1}{3}<\alpha<1, \tag{2.9}$$

and $\varphi\in C^\infty(\mathbb{R})$ with $\varphi(y)=0$ for $y\leqq 0$, $\varphi(y)=1/2$ for $y\geqq 1$ and $\varphi'(y)\geqq 0$.

The set in which $f_k(t,x)$ depends on x, i.e., $\nabla_x f(t,x)\neq 0$, is contained in

$$M_k(t)=\left\{x\in\mathbb{R}^\nu \mid 0<w_k\cdot\frac{x}{t}-w_k^2<\frac{1}{t^{1-\alpha}}\right\}. \tag{2.10}$$

For $w_k\cdot\frac{x}{t}\leqq w_k^2$ the function $f_k(t,x)$ vanishes and gives no contribution to $B(t)$. On the other hand, we get inside $\left\{x \mid w_k\cdot\frac{x}{t}\geqq w_k^2+\frac{1}{t^{1-\alpha}}\right\}$ that $f_k(t,x)=\frac{1}{2}$. According to the beginning of this section, this means in the case $\lambda_k(t)=\lambda_k$, $M=1$, that the operator $B(t)$ measures the energy in this region in a Galilei-system moving with the velocity $\lambda_k w_k$. Thus, $M_k(t)$ defines a boundary between these two areas of different energy measurement.

Because there are only finitely many w_k and v_j, (2.1) implies that there are neighborhoods U_j of v_j and some $\delta > 0$, such that

$$|w_k \cdot v - w_k^2| > \delta \tag{2.11}$$

for all k, j, and $v \in U_j$. Hence the sets $t \cdot U_j = \left\{ x \mid \frac{x}{t} \in U_j \right\}$ are disjoint from the boundaries $M_k(t)$ for large t. With Lemma 2.1, we can find a $t_0 > 0$ and a neighborhood U of the origin, such that

$$M_k(t) \cap \{y_j(t) + tv \mid v \in U\} = \emptyset \quad \text{for all } t \geqq t_0, j, k. \tag{2.12}$$

The next lemma shows that $A(t)$ satisfies the condition which we want to have. Taking $P^{(k)}$ instead of P gives better control of the terms due to the boundaries $M_k(t)$.

Lemma 2.2. *There is a $t_0 > 0$ and a neighborhood U of the origin, such that*

$$2 \cdot \sum_{k=1}^{M} \lambda_k(t) w_k f_k(t, x) = \dot{y}_j(t) \tag{2.13}$$

for all j, $t \geqq t_0$, and $x \in \{y_j(t) + tv \mid v \in U\}$.

Proof. With (2.12), we have already shown that for a fixed j, the function $f_k(t, x)$ can only take the two values 0 and $\frac{1}{2}$, depending on which side of $M_k(t)$ the set $\{y_j(t) + tv \mid v \in U\}$ lies. Thus (2.13) follows from (2.2). □

The next step consists of the computation of the time derivative of $B(t)$.

Lemma 2.3. *There exists a $t_0 > 0$ such that for $\psi \in D(H_0)$, $s \in \mathbb{R}$, $t \geqq t_0$, and $\psi(t) = U(t, s)\psi$ the scalar product $(\psi(t), B(t)\psi(t))$ is continuously differentiable and*

$$\frac{d}{dt}(\psi(t), B(t)\psi(t))$$

$$= -\frac{2}{mt^\alpha} \sum_{k=1}^{M} \lambda_k(t) \left\| [\varphi'(\xi_k)]^{1/2} \left(w_k \cdot P^{(k)} - \frac{m\alpha}{2} t^{\alpha - 1} \xi_k \right) \psi(t) \right\|^2 \tag{2.14}$$

$$+ 2 \,\mathrm{Re} \sum_{k=1}^{M} (h_k(t, x)\psi(t), P^{(k)}\psi(t)) \tag{2.15}$$

$$+ \sum_{n=1}^{3} (\psi(t), g_n(t, x)\psi(t)), \tag{2.16}$$

where

$$\xi_k = t^{-\alpha} w_k \cdot [x - t w_k],$$

$$h_k(t, x) = -\dot{\lambda}_k(t) w_k f_k(t, x),$$

$$g_1(t, x) = \sum_{j=1}^{N} \left[2 \sum_{k=1}^{M} \lambda_k(t) w_k f_k - \dot{y}_j(t) \right] (\nabla V_j)(x - y_j(t)),$$

$$g_2(t, x) = \sum_{k=1}^{M} \frac{m\alpha^2}{2t^{2-\alpha}} \lambda_k(t) \xi_k^2 \varphi'(\xi_k),$$

$$g_3(t, x) = \sum_{k=1}^{M} \frac{\lambda_k(t)}{2m} \frac{|w_k|^4}{t^{3\alpha}} \varphi'''(\xi_k).$$

Proof. The potentials $V_j(x-y_j(t))$ are contained in $B(t)$ and we have to use

$$(\psi(t), V_j(x-y_j(t))\psi(t)) = (\tilde{\psi}(t), V_j(x)\tilde{\psi}(t)), \tilde{\psi}(t) = e^{iy_j(t)\cdot P}\psi(t), \tag{2.17}$$

for the time derivative, if $i[P, V_j(x)] = \nabla V_j(x)$ is not H_0-bounded. For the sake of simplicity we only consider the formal derivative

$$\begin{aligned} i[H(t), B(t)] + \frac{\partial}{\partial t} B(t) &= -i[H(t), A(t)] + \frac{\partial}{\partial t} H(t) - \frac{\partial}{\partial t} A(t) \\ &= \sum_{j=1}^{N} \left(-i[V_j(x-y_j(t)), A(t)] + \frac{\partial}{\partial t} V_j(x-y_j(t))\right) \\ &\quad -i[H_0, A(t)] - \frac{\partial}{\partial t} A(t). \end{aligned}$$

The first sum on the right side of the last equality gives $g_1(t,x)$, which is bounded if we take t_0 large enough (see Lemma 2.2).

For the computation of $-i[H_0, A(t)]$, we use

$$i[H_0, f_k] = \frac{P}{m}(\nabla f_k) + \frac{i}{2m}(\Delta f_k) = (\nabla f_k)\frac{P}{m} - \frac{i}{2m}(\Delta f_k)$$

and

$$\nabla f_k = \varphi'(\xi_k) t^{-\alpha} w_k, \qquad \Delta f_k = \varphi''(\xi_k) t^{-2\alpha} w_k^2.$$

Thus we get

$$\begin{aligned} -i[H_0, A(t)] = &- \sum_{k=1}^{M} \lambda_k(t) w_k \cdot \left\{ \frac{P\cdot w_k}{mt^\alpha} \varphi'(\xi_k) P^{(k)} + P^{(k)}\varphi'(\xi_k)\frac{w_k\cdot P}{mt^\alpha}\right\} \\ &- \sum_{k=1}^{M} \lambda_k(t) w_k \frac{i}{2m}\left[\frac{w_k^2}{t^{2\alpha}}\varphi''(\xi_k), P^{(k)}\right], \end{aligned}$$

where the last sum is $g_3(t,x)$. With

$$\frac{\partial}{\partial t} f_k = \varphi'(\xi_k)\left[-\frac{\alpha}{t}\xi_k - \frac{w_k^2}{t^\alpha}\right],$$

we have

$$\begin{aligned} -\frac{\partial}{\partial t} A(t) = &\sum_{k=1}^{M} \{h_k(t,x)P^{(k)} + P^{(k)}h_k(t,x)\} \\ &- \sum_{k=1}^{M} \lambda_k(t) w_k \left\{\left[-\frac{w_k^2}{t^\alpha} - \frac{\alpha}{t}\xi_k\right]\varphi'(\xi_k)P^{(k)} + P^{(k)}\varphi'(\xi_k)\left[-\frac{w_k^2}{t^\alpha} - \frac{\alpha}{t}\xi_k\right]\right\}. \end{aligned}$$

The proof is finished with the following equality:

$$\begin{aligned} &- \sum_{k=1}^{M} \lambda_k(t) w_k \left\{\frac{P\cdot w_\alpha}{mt^\alpha}\varphi'(\xi_k)P^{(k)} + P^{(k)}\varphi'(\xi_k)\frac{w_k\cdot P}{mt^\alpha}\right\} \\ &- \sum_{k=1}^{M} \lambda_k(t) w_k \left\{\left[-\frac{w_k^2}{t^\alpha} - \frac{\alpha}{t}\xi_k\right]\varphi'(\xi_k)P^{(k)} + P^{(k)}\varphi'(\xi_k)\left[-\frac{w_k^2}{t^\alpha} - \frac{\alpha}{t}\xi_k\right]\right\} \\ = &- \sum_{k=1}^{M} \frac{2}{mt^\alpha}\lambda_k(t)\left(w_k\cdot P^{(k)} - \frac{m\alpha}{2}t^{\alpha-1}\xi_k\right)\varphi'(\xi_k)\left(w_k P^{(k)} - \frac{m\alpha}{2}t^{\alpha-1}\xi_k\right) \\ &+ g_2(t,x). \quad \square \end{aligned}$$

By (2.4) the functions $\lambda_k(t)$ are positive for large t, and thus (2.14) is negative for states $\psi(t)$ crossing one of the boundaries $M_k(t)\,(\supset \operatorname{supp}\varphi'(\xi_k))$. This represents a kind of energy loss as the particle scatters from one center of force to another. This feature is important for the proof of asymptotic completeness for the charge transfer model in [9].

Due to the fact that the rest frames of the heavy particles are not necessarily inertial, we get (2.15). If the forces $\nabla V_j(x-y_j(t))$ cannot be separated by the $M_k(t)$, we have to deal with their tails. This gives $g_1(t,x)$. The function $g_3(t,x)$ is a pure quantum effect. A quantum state does not like to have its position measured precisely. Thus we have taken an increasing thickness t^α of $M_k(t)$. The time dependence of the thickness causes the $\frac{m\alpha}{2}t^{\alpha-1}\xi_k$ in (2.14) and the additional term $g_2(t,x)$.

From Lemma 2.2 Assumption 4 and (2.9), we get

$$\sum_{n=1}^{3}(\psi(t), g_n(t,x)\psi(t))\in L^1([t_0,\infty), dt).$$

Furthermore, we can estimate (2.15) by

$$2\sum_{k=1}^{M}\|h_k(t,x)\psi(t)\|\cdot(\|P\psi(t)\|+\|mw_k\psi(t)\|).$$

Using (2.3), we obtain the following.

Corollary 2.4. *For some $t_0>0$, there are functions $g,h\in L^1([t_0,\infty),dt)$ such that*

$$\frac{d}{dt}(\psi(t), B(t)\psi(t))\leqq g(t)+h(t)\,\|P\psi(t)\|\,.$$

It is easily seen from the definition that $A(t)$ is form bounded with respect to H_0 with form bound zero uniformly in $t>0$. Hence, for every $a>0$ there is a $b\in\mathbb{R}_+$ such that

$$\frac{1}{2m}\|P\varphi\|^2=(\varphi,H_0\varphi)\leqq(\varphi,B(t)\varphi)+a(\varphi,H_0\varphi)+b\,\|\varphi\|^2$$

for all $\varphi\in Q(H_0)$. By Corollary 2.4, we get

$$\begin{aligned}\frac{1-a}{2m}\sup_{t_0\leqq t\leqq T}\|P\psi(t)\|^2 &\leqq \sup_{t_0\leqq t\leqq T}(\psi(t),B(t)\psi(t))+b\,\|\psi\|^2\\ &\leqq \mathrm{const}_{t_0}+\int_{t_0}^{T}dt\,h(t)\,\|P\psi(t)\|\end{aligned}$$

with

$$\mathrm{const}_{t_0}=(\psi(t_0),B(t_0)\psi(t_0))+\int_{t_0}^{\infty}dt\,g(t)+b\,\|\psi\|^2\,.$$

If $\sup_{t_0\leqq t\leqq T}\|P\psi(t)\|^2\leqq 1$ for all $T\geqq t_0$, then the proof of Theorem 1.1 is finished. Otherwise we can divide by $\sup_{t_0\leqq t\leqq T}\|P\psi(t)\|$, which also proves the statement, since h is integrable.

3. Geometry of the Boundaries

In this section we show the existence of the w_k and $\lambda_k(t)$, $k=1,\dots,M$, which we have needed for the definition of $B(t)$. They are not determined by (2.1)–(2.4), and we have a great deal of freedom in choosing them. First we take an orthonormal basis $\{e_i\}_{i=1,\dots,\nu}$ of $\mathbb{R}^\nu$ with

$$v_{ji} \neq v_{li} \tag{3.1}$$

for $j \neq l$, $i=1,\dots,\nu$, where we have defined

$$v_{ji} = e_i \cdot v_j .$$

Furthermore, we assume that for all j and i

$$v_{ji} > 0 . \tag{3.2}$$

This is not really necessary, but it simplifies the notation, and it is possible to get (3.2) by a Galilei-transformation. So we have no loss of generality.

Lemma 3.1. *There are finitely many $w_k \in \mathbb{R}^\nu$ and $\lambda_k(t)$, $k=1,\dots,M$, satisfying* (2.1)–(2.4).

Proof. If is sufficient to find $w_k \in \mathbb{R}^\nu \setminus \{0\}$, $\lambda_k(t)$ with

$$\sum_{\substack{k \\ w_k \cdot v_j \geqq w_k^2}} \lambda_k(t) w_k = \dot{y}_j(t), \quad j=1,\dots,N, \tag{3.3}$$

instead of (2.1) and (2.2), because in the case of $w_k \cdot v_j = w_k^2$ we get for $\tilde{w}_k = (1-\varepsilon) w_k$, $\varepsilon > 0$, the inequality $\tilde{w}_k \cdot v_j > \tilde{w}_k^2$. We have to choose ε small enough to preserve $w_k \cdot v_l < w_k^2$, if this occurs for some l. Of course, we will scale $\lambda_k(t)$ with $(1-\varepsilon)^{-1}$, since we want to have the same product $\lambda_k(t) w_k$.

We will take $(i,n) \in \{1,\dots,\nu\} \times \{1,\dots,N\}$ instead of $k \in \{1,\dots,M\}$ and

$$w_k = w_{i,n} = a_{i,n} e_i , \qquad a_{i,n} > 0 .$$

Hence (3.3) is equivalent to

$$\sum_{\substack{n \\ v_{ji} \geqq a_{i,n}}} \lambda_{i,n}(t) a_{i,n} = e_i \cdot \dot{y}_j(t), \quad \text{for all } i \text{ and } j . \tag{3.4}$$

For the idea of this procedure, see the example behind the proof. We fix $i \in \{1,\dots,\nu\}$ and sort the set $\{v_{1,i},\dots,v_{N,i}\}$, i.e., there is a permutation μ of $\{1,\dots,N\}$ such that

$$0 < v_{\mu(1),i} < v_{\mu(2),i} < \dots < v_{\mu(N),i} . \tag{3.5}$$

Define

$$a_{i,n} = v_{\mu(n),i} ,$$

and

$$\lambda_{i,n}(t) = \begin{cases} \dfrac{1}{a_{i,n}} e_i \cdot (\dot{y}_{\mu(n)}(t) - \dot{y}_{\mu(n-1)}(t)) & \text{for} \quad n > 1 \\ \dfrac{1}{a_{i,1}} e_i \cdot \dot{y}_{\mu(1)}(t) & \text{for} \quad n = 1 . \end{cases}$$

For fixed j and $j' = \mu^{-1}(j)$, we get

$$\sum_{\substack{n \\ v_{ji} \geqq a_{i,n}}} \lambda_{i,n}(t) a_{i,n} = \sum_{n=1}^{j'} \lambda_{i,n}(t) a_{i,n} = e_i \cdot \dot{y}_j(t).$$

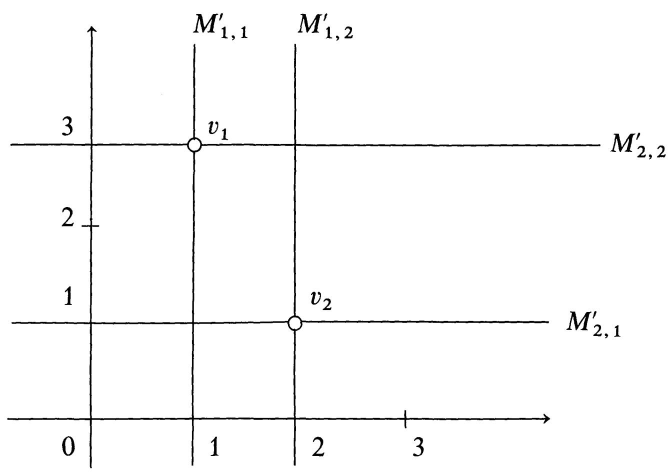
Obviously, (2.3) and (2.4) follow from Assumption (1) and (3.5). □

Since the proof perhaps does not make the idea of choosing the w_k and $\lambda_k(t)$ clear enough, we will consider the example: $N=2$, $v=2$, $\dot{y}_1(t) = v_1 = (1,3)$ and $\dot{y}_2(t) = v_2 = (2,1)$. The points v_1 and v_2 are in velocity space, which simultaneously should be thought of as position space divided by the time. The thickness of the boundaries $M_k(t)$ [see (2.10)] is here $t^{-1+\alpha}$, which goes to zero for $t \to \infty$. For the sake of simplicity we will assume we have sharp boundaries $M'_k = \{v | w_k \cdot v = w_k^2\}$. The procedure of the proof gives

$$w_{1,1} = (1,0), \quad w_{1,2} = (2,0), \quad w_{2,1} = (0,1), \quad w_{2,2} = (0,3),$$

which leads to the boundaries

$$M'_{1,1} = \{(1,\mu) | \mu \in \mathbb{R}\}, \quad M'_{1,2} = \{(2,\mu) | \mu \in \mathbb{R}\},$$
$$M'_{2,1} = \{(\mu,1) | \mu \in \mathbb{R}\}, \quad M'_{2,2} = \{(\mu,3) | \mu \in \mathbb{R}\}.$$



We can see from the definition (2.5)–(2.9) that $B(t) = H(t)$ near the origin. To find out whether $B(t)$ measures the energy at the first center of force in the right Galilei system (= rest frame of this center), we have to sum up all changes at the boundaries between the origin and v_1. By the scaling with $(1-\varepsilon)$ the boundaries M'_k with $v_1 \in M'_k$ have to be included. These are $M'_{1,1}$, $M'_{2,1}$, and $M'_{2,2}$. While the w_k determines the site of the boundaries, the velocity difference of the Galilei systems on both sides of a boundary M'_k is $\lambda_k w_k$. Here $\lambda_{1,1} = 1$, $\lambda_{1,2} = 1/2$, $\lambda_{2,1} = 1$, and $\lambda_{2,2} = 2/3$. Therefore, the velocity of the Galilei system, in which the energy is measured at v_1, is given by

$$\lambda_{1,1} w_{1,1} + \lambda_{2,1} w_{2,1} + \lambda_{2,2} w_{2,2} = v_1 .$$

This equation is (3.3) for $j=1$.

4. Corollaries

If the particle travels with bounded speed, the position divided by the time will be bounded, too. For time independent Hamilton operators, this is shown in [6] with a similar proof.

Corollary 4.1. *Let* $D=D(H_0)\cap D(|x|)$. *Then*

(a) $U(t,s)D=D \quad \text{for } t,s\in\mathbb{R},$ (4.1)

(b) $\sup_{t\geqq s}\left(\psi(t),\frac{x^2}{1+t^2}\psi(t)\right)<\infty$ (4.2)

for each $\psi\in D$, $s\in\mathbb{R}$, *and* $\psi(t)=U(t,s)\psi$.

Proof. We define $x_\varepsilon=x(1+\varepsilon x^2)^{-1/2}$ and compute

$$i[H(t),x_\varepsilon^2]=i[H_0,x_\varepsilon^2]=\frac{1}{2m}\{P\cdot\nabla x_\varepsilon^2+\nabla x_\varepsilon^2\cdot P\}$$

$$=\frac{1}{m}\{P\cdot(1+\varepsilon x^2)^{-3/2}x_\varepsilon+x_\varepsilon(1+\varepsilon x^2)^{-3/2}\cdot P\}.$$

Hence, for $s\in\mathbb{R}$, $T\geqq s$, $\psi\in D$, and $\psi(t)=U(t,s)\psi$, we get

$$\sup_{t\in[s,T]}\|x_\varepsilon\psi(t)\|^2\leqq\|x_\varepsilon\psi\|^2+\int_s^T dt|(\psi(t),i[H(t),x_\varepsilon^2]\psi(t))|$$

$$\leqq\|x_\varepsilon\psi\|^2+\frac{2|T-s|}{m}\sup_{t\in[s,T]}\|P\psi(t)\|\cdot\sup_{t\in[s,T]}\|x_\varepsilon\psi(t)\|. \quad (4.3)$$

In the case $T\leqq s$, we get the same inequality for $\sup_{t\in[T,s]}\|x_\varepsilon\psi(t)\|$. This shows that $\||x|(1+\varepsilon x^2)^{-1/2}\psi(t)\|=\|x_\varepsilon\psi(t)\|$ has a bound independent of ε, and

$$U(t,s)\psi=\lim_{\varepsilon\to 0}(1+\varepsilon x^2)^{-1/2}\psi(t)\in D$$

for every $t\in\mathbb{R}$. It follows that $U(t,s)D\subset D$, $D=U(t,s)\,[U(s,t)D]\subset U(t,s)D$, and thus (4.1). Taking $\varepsilon=0$ in (4.3) implies

$$\|x\psi(T)\|\leqq\|x\psi\|+\frac{2|T-s|}{m}\sup_{t\geqq s}\|P\psi(t)\|\leqq\text{const}_{\psi,s}(1+|s|+|T|). \quad \square$$

Corollary 4.2. *Let* $s\in\mathbb{R}$, $\psi\in\mathscr{H}$, *and* $\psi(t)=U(t,s)\psi$. *Then*

(a) $\lim_{E\to\infty}\sup_{t\geqq s}\|F(H(t)\geqq E)\psi(t)\|=0,$

(b) $\lim_{E\to\infty}\sup_{t\geqq s}\|F(H_0\geqq E)\psi(t)\|=0,$

(c) $\lim_{v\to\infty}\sup_{t\geqq s}\|F(|x|\geqq v(|t|+1))\psi(t)\|=0.$

Proof. Since the projectors and the propagator are uniformly bounded, it is sufficient to prove the statements for $\psi\in D$. Using (1.5), the norm in (a) is bounded by

$$\|F(H(t)\geqq E)(H(t)+M)^{-1/2}\|\cdot\|(H(t)+M)^{1/2}\psi(t)\|.$$

Because the second factor is bounded in $t \geqq s$, the first one gives the convergence. The proofs of (b) and (c) are similar. □

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