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Distortion analyticity and molecular resonance curves

by

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ABSTRACT. — Resonance energies of n electrons in the field of N fixed nuclei are defined as discrete eigenvalues of non-selfadjoint operators which arise from the Hamiltonian H by a general class of complex distortions of R^3 around the fixed nuclei. They are identified with the poles in the analytic continuation of resolvent matrix-elements $(\varphi, (z - H)^{-1}\psi)$ between states φ, ψ of an explicitely given set A of analytic vectors, and thus shown to be independent of the particular choice of the distortion. Distortions are also used to derive local analyticity properties of bound state-and resonance energies in the nuclear coordinates.

RÉSUMÉ. — On définit les énergies de résonances de n électrons dans le champ de N noyaux fixes comme valeurs propres discrètes d'opérateurs non auto-adjoints obtenus à partir du Hamiltonien H par une classe générale de déformations complexes de R^3 autour des noyaux fixes. On identifie ces énergies avec les pôles des prolongements analytiques des éléments de matrice de la résolvante $(\phi, (z - H)^{-1}\psi)$ entre des états ϕ, ψ d'un ensemble A de vecteurs analytiques donné explicitement, montrant ainsi qu'elles sont indépendantes du choix particulier de la déformation. On utilise aussi ces déformations pour démontrer des propriétés d'analyticité locale des énergies d'états liés et de résonances par rapport aux coordonnées de noyaux.

1. INTRODUCTION

$$H(X) = \sum_{i=1}^{n} \left(p_i^2 - \sum_{r=1}^{N} Z_r \, | x_i - X_r |^{-1} \right) + \sum_{i<k}^{1 \ldots n} | x_i - x_k |^{-1} \tag{1}$$

is the Hamiltonian of n electrons in the external field of N nuclei fixed in the configuration $X = (X_1 \ldots X_N) \in R^{3N}$. We will discuss H(X) as an operator on $L^2(R^{3n})$, since the Pauli principle is not relevant in the present context. Our goal is to define « resonances » associated with H(X) and to analyze their local behavior as functions of X.

Resonances appear in the standard form of the Balslev-Combes theory [*2*] [*10*] as discrete eigenvalues of a family of non-selfadjoint operators $H(\theta)$, which arises from the Hamiltonian H by the group of dilations

$$x_i \to e^{\theta} x_i \tag{2}$$

and which is then continued analytically in the group parameter θ. Except for the case of « atoms » ($N = 1, X = 0$), this procedure fails in the case of H(X): the transformed Hamiltonian $H(X, \theta)$ is not dilation analytic for the simple reason that the potentials $| e^{\theta} x_i - X_r |^{-1}$ are not analytic in θ if $X_r \neq 0$. Simon [*12*] has resolved this difficulty by the device of « exterior complex scaling », where (2) is replaced by the group

$$x_i \to x_i f_\theta(| x_i |) \tag{3}$$

$$f_\theta(r) = \begin{cases} 1 & ; 0 \leq r \leq R \\ r^{-1}(R + e^{\theta}(r - R)); & R \leq r < \infty . \end{cases}$$

Here R is chosen so large that

$$| X_r | < R ; \qquad r = 1 \ldots N. \tag{4}$$

As a consequence, the Coulomb singularities at $x_i = X_r$ are not displaced by (3), so that the transformed Hamiltonian $H(X, \theta)$ is analytic in the group parameter θ. It is then possible to to construct the resonances along the lines of the Balslev-Combes theory, and it turns out that they are independent of the particular choice of R. Alternative methods to deal with non dilation-analytic potentials have been developed by Sigal [*11*] and Cycon [*4*]. These authors use maps in momentum space, with the consequence that the transformed Hamiltonians are no longer local.

In this paper we generalize (3) to a class of distortions

$$x_i \to x_i + \lambda v(x_i) , \tag{5}$$

where $v(x)$ is a fixed but largely arbitrary smooth vector field $R^3 \to R^3$,

and λ distortion parameter taking over the role of the group parameter θ. The required properties of $v(x)$ are:

$$|v(x) - v(y)| \leq |x - y|, \tag{6}$$

$$v(X_r) = 0; \qquad r = 1 \ldots N, \tag{7}$$

$$v(x) = x \quad \text{for sufficiently large } |x|. \tag{8}$$

By (6) the map (5) is invertible for real λ with $|\lambda| < 1$ and thus induces a unitary operator $U(\lambda)$ on $L^2(R^{3n})$. (7) states that the Coulomb singularities $|x_i - X_r|^{-1}$ are not displaced under (5). As a consequence, the family of distorted Hamiltonians

$$H(X, \lambda) = U(\lambda)H(X)U(\lambda)^{-1}, \tag{9}$$

$(-1 < \lambda < +1)$ has an analytic continuation to the complex disc $|\lambda| < 2^{-\frac{1}{2}}$. (8) is used to control the essential spectrum of $H(X, \lambda)$ as in the dilation-analytic case.

In contrast to (2) and (3) the maps (5) and the corresponding unitary operators $U(\lambda)$ do not form a group. We could of course preserve the group structure by considering the flow generated in R^3 by the vector field $v(x)$, but we find it more convenient to work with the explicit form (5). As has been remarked by Cycon [4], it is possible to save the Balslev-Combes argument without the group property by constructing a sufficiently large set A of analytic vectors, i. e. wave functions $\psi(x_1 \ldots x_n)$ for which

$$\lambda \to \psi(x_1 + \lambda v(x_1), \ldots, x_n + \lambda v(x_n))$$

is analytic as an L^2-valued function in the disc $|\lambda| < 2^{-\frac{1}{2}}$. This set A will be the same for all admissible vector fields $v(x)$, and the resonances (i. e. the complex discrete eigenvalues of $H(X, \lambda)$) can be identified with the poles of the functions $z \to (\varphi, (z - H(X))^{-1}\psi)$; $\varphi, \psi \in A$; analytically continued across the continuous spectrum of $H(X)$. This shows that the resonances are characterized by the pair $H(X)$, A: they are independent of λ and of the particular choice of $v(x)$.

The theory outlined above is developed in the present paper. In addition, we use the machinery of distortions to derive local analyticity properties of bound state-and resonance energies in the nuclear coordinates $X_1 \ldots X_n$. These results are of interest in connection with the Born-Oppenheimer approximation [8].

2. DISTORTIONS OF R^3

Let $v(x)$ be a C^∞-vector field $R^3 \to R^3$ satisfying

$$|v(x) - v(y)| \leq L|x - y|; \qquad L < 1. \tag{10}$$

Then the map

$$x \to x + v(x) \equiv y(x) \tag{11}$$

is invertible: for any $y \in \mathrm{R}^3$, x is given by the limit $n \to \infty$ of $x_n = y - v(x_{n-1})$, $x_0 = y$. The Jacobian of (11) is

$$\mathrm{J}_{ik}(x) = \delta_{ik} + v_{i,k}(x), \tag{12}$$

with the matrix $v_{i,k} \equiv \partial v_i / \partial x_k$ satisfying

$$\| v_{i,k}(x) \| \leq \mathrm{L} < 1, \tag{13}$$

as an operator on R^3. In particular, the eigenvalues of the matrix $v_{i.k}$ have absolute values $\leq \mathrm{L}$ so that

$$\mathrm{J}(x) \equiv \det (\mathrm{J}_{ik}(x)) \geq (1 - \mathrm{L})^3 > 0. \tag{14}$$

We conclude that (11) is in fact a C^∞-diffeomorphism of R^3 onto R^3.

3. THE DISTORTED HAMILTONIAN

On the one-electron Hilbert space $\mathrm{L}^2(\mathrm{R}^3)$ the map (11) induces the unitary transformation

$$(\mathrm{U}\psi)(x) = \mathrm{J}^{\frac{1}{2}}(x)\psi(x + v(x)), \tag{15}$$

and on the n-electron Hilbert space $\mathrm{L}^2(\mathrm{R}^{3n})$ the corresponding tensor product

$$(\mathrm{U}\psi)(x_1 \ldots x_n) = \mathrm{J}^{\frac{1}{2}}(x_1) \ldots \mathrm{J}^{\frac{1}{2}}(x_n)\psi(x_1 + v(x_1), \ldots, x_n + v(x_n)). \tag{16}$$

The one-electron kinetic energy $p^2 = -\Delta$ on $\mathrm{L}^2(\mathrm{R}^3)$ transforms under (15) according to

$$\mathrm{U}p^2\mathrm{U}^{-1} = \mathrm{J}^{-\frac{1}{2}}p_i\mathrm{J}^{ik}\mathrm{J}\mathrm{J}^{mk}p_m\mathrm{J}^{-\frac{1}{2}} \equiv \mathrm{T}(x, p), \tag{17}$$

with sums over all double indices i, k, m. Here $p_1 \ldots p_3$ are the momentum operators $p_i = -i\partial/\partial x_i$ and (J^{ik}) is the inverse of the matrix (J_{ik}). For the transformed potentials we find

$$\begin{aligned} \mathrm{U} \,|\, x_i - \mathrm{X}_r \,|^{-1}\mathrm{U}^{-1} &= |\, x_i + v(x_i) - \mathrm{X}_r \,|^{-1}, \\ \mathrm{U} \,|\, x_i - x_k \,|^{-1}\mathrm{U}^{-1} &= |\, x_i - x_k + v(x_i) - v(x_k) \,|^{-1}. \end{aligned} \tag{18}$$

4. ANALYTICITY OF BOUND STATE ENERGIES IN THE NUCLEAR COORDINATES

As a first application of distortions we show that analytic perturbation theory with respect to X is applicable to the discrete eigenvalues of H(X) despite the fact that H(X) is not an analytic family.

THEOREM 1. — *Let* $X \in R^{3N}$ *be fixed with*

$$X_r \neq X_s \qquad \text{if} \qquad r \neq s. \tag{19}$$

For small $\xi \in R^{3N}$ *we then have*

$$H(X + \xi) = U^{-1}(\xi)\tilde{H}(\xi)U(\xi), \tag{20}$$

where $U(\xi)$ *is unitary and where* $\tilde{H}(\xi)$ *is an analytic family of type* A *for small* $\xi \in C^{3N}$.

Proof. — By (19) we can pick real $C_0{}^\infty$-functions $f_1 \ldots f_N$ on R^3 such that

$$f_r(X_s) = \delta_{rs}. \tag{21}$$

For any $\xi = (\xi_1 \ldots \xi_N) \in R^{3N}$ we then define the vector field

$$v(x) = \sum_{r=1}^{N} \xi_r f_r(x), \tag{22}$$

which satisfies (10) for small ξ and interpolates the prescribed values

$$v(X_r) = \xi_r; \qquad r = 1 \ldots N. \tag{23}$$

Let $U(\xi)$ be the unitary operator (16) for this vector field. Due to (23) the transformed potentials (18) can all be represented by the same function

$$V(x, y) = |x - y + v(x) - v(y)|^{-1} = (1 + w)^{-\frac{1}{2}} |x - y|^{-1}, \tag{24}$$

$$\omega = |x - y|^{-2}[2(x - y, v(x) - v(y)) + (v(x) - v(y), v(x) - v(y))]. \tag{25}$$

The transformed Hamiltonian is

$$\tilde{H}(\xi) = U(\xi)H(X + \xi)U(\xi)^{-1}$$

$$= \sum_{i=1}^{n}\left[T(x_i, p_i) - \sum_{r=1}^{N} Z_k V(x_i, X_r)\right] + \sum_{i<k}^{1\ldots n} V(x_i, x_k), \tag{26}$$

with $T(x, p)$ given by (17). These explicit expressions also define $\tilde{H}(\xi)$ for small complex $\xi \in C^{3N}$. Then $v(x)$ is a complex vector field, linear in ξ, which vanishes uniformly in x with all its derivatives as $\xi \to 0$. In particular (10) and (13) hold in the sense of the norm on C^3 with $L < \sqrt{2} - 1$ for sufficiently small ξ. It then follows from (25) that $|w| \leq 2L + L^2 < 1$, so that the factors $(1 + w)^{-\frac{1}{2}}$ in the potentials are bounded multiplication operators analytic in ξ. The remaining factors are the undistorted Coulomb potentials: they are independent of ξ and have arbitrarily small relative bound with respect to

$$p^2 \equiv p_1^2 + \ldots + p_n^2 \qquad \text{on} \qquad L^2(R^{3n}).$$

For small $\xi \in C^{3N}$ the one-particle kinetic energy (17) has the form

$$T(x, p) = p^2 + a_{ik}(x)p_i p_k + a_i(x)p_i + a(x)$$

on $L^2(R^3)$, where the a's are bounded multiplication operators, analytic in ξ, which vanish in norm as $\xi \to 0$. We thus conclude that for small $\xi \in C^{3N}$

$$\tilde{H}(\xi) = p^2 + A(\xi),$$

where $A(\xi)$ is analytic in ξ as a bounded operator from $D(p^2)$ (equipped with the norm $\| \psi \| + \| p^2\psi \|$) to $L^2(R^{3n})$ and satisfies an estimate

$$\| A(\xi)\psi \| \leq \alpha \| p^2\psi \| + \beta \| \psi \|$$

with $\alpha < 1$. Therefore $\tilde{H}(\xi)$ is an analytic family of type A in some neighbourhood of $\xi = 0$. ■

COROLLARY. — *Nondegenerate discrete eigenvalues of* $H(X)$ *are analytic in* $X \in C^{3N}$ *in a neighbourhood of any nuclear configuration* $X \in R^{3N}$ *satisfying (19).*

Remarks. — The corollary follows directly from (20) since $H(X + \xi)$ and $\tilde{H}(\xi)$ have the same spectrum for small $\xi \in R^{3N}$. Non-degeneracy is essential for analyticity of eigenvalues in several complex variables. A standard example is the 2×2 matrix

$$\begin{pmatrix} \xi_1 & \xi_2 \\ \xi_2 & -\xi_1 \end{pmatrix}$$

which is an entire function of $\xi \in C^2$ and has the eigenvalues $\pm (\xi_1^2 + \xi_2^2)^{\frac{1}{2}}$, which are not jointly analytic in (ξ_1, ξ_2) at $\xi_1 = \xi_2 = 0$. There is no reason to expect that this phenomenon cannot occur for degenerate eigenvalues of $H(X)$.

In the case $N = 2$ we can adapt the coordinate system so that $X_1 = 0$ and $X_2 = (r, 0, 0)$, which shows that the spectrum of $H(X)$ depends only on the single variable $r = | X_1 - X_2 |$. Analyticity in r of discrete eigenvalues near any $r > 0$ was already proven in [*1*]. It is also known that analyticity breaks down in a very subtle way at $r = 0$: for H_2^+ ($N = 2$, $n = 1$) the electronic ground state energy has an expansion of the form

$$E(r) = c_0 + c_2 r^2 + c_3 r^3 + c_4 r^4 + c_5 r^5 \log r + O(r^5)$$

as $r \to 0$ [*9*]. This shows that the condition (19) is not redundant.

In general (for any N, n, for arbitrary nuclear configurations X and without regard to degeneracies) it is only known that the eigenvalues of $H(X)$ satisfy a Lipschitz inequality

$$| E_k(X) - E_k(Y) | \leq c \| X - Y \|,$$

where $\| \ \|$ is a norm on R^{3N} and c a constant independent of X, Y, which can be estimated in terms of the parameters of the model. Here $E_k(X)$

is the k'th eigenvalue counted from the bottom of the spectrum, or the bottom of the continuous spectrum if the total multiplicity of the discrete eigenvalues of H(X) is less than k [7].

5. THE FAMILY $H(X, \lambda)$

In this section we define the distorted Hamiltonians (9) which will be used to construct the resonances. Let $v(x)$ be a C^∞-vector field $R^3 \to R^3$ satisfying (6) and (7). For real λ with $|\lambda| < 1$ the map

$$x \to x + \lambda v(x), \tag{27}$$

is then a C^∞-diffeomorphism of R^3 onto R^3. Let $U(\lambda)$ be the corresponding unitary operator (16), where $v(x)$ is now to be replaced by $\lambda v(x)$. (7) is used to rewrite the distorted nuclear potential as

$$U(\lambda)\,|x_i - X_r|^{-1} U(\lambda)^{-1} = |x_i - X_r + \lambda v(x_i) - \lambda v(X_r)|^{-1}.$$

The transformed Hamiltonian $H(X, \lambda) = U(\lambda)H(X)U(\lambda)^{-1}$ is then given by (26), provided that $\lambda v(x)$ is substituted for $v(x)$ wherever it occurs. This explicit expression now defines $H(X, \lambda)$ for complex λ in the disc $|\lambda| < 1$ as an operator with domain $D(p^2)$: the potential (24) has the form

$$V(x, y) = \left[\left(\frac{x-y}{|x-y|} + \lambda \frac{v(x) - v(y)}{|x-y|}\right)^2\right]^{-\frac{1}{2}} \frac{1}{|x-y|}, \tag{28}$$

so that by (6)

$$|V(x, y)| \leq (1 - |\lambda|)^{-1}\,|x - y|^{-1}. \tag{29}$$

The kinetic energy (17) is well defined since the (real) matrix $v_{i,k}$ satisfies

$$\| v_{i,k}(x) \| \leq 1 \tag{30}$$

as an operator on C^3. Therefore the Jacobian

$$J_{ik}(x) = \delta_{ik} + \lambda v_{i,k}(x) \tag{31}$$

has a determinant $J(x)$ bounded away from zero by

$$|J(x)| \geq (1 - |\lambda|)^3. \tag{32}$$

THEOREM 2. — *Let $v(x)$ be a C^∞-vector field $R^3 \to R^3$ with bounded derivatives satisfying (6)(7). Then for*

$$|\lambda| \leq 2^{-\frac{1}{2}} - \varepsilon \qquad (\varepsilon > 0) \tag{33}$$

$H(X, \lambda)$ is m-sectorial with a sector

$$S = \left\{ z \,|\, |\arg(z - a)| \leq b < \frac{\pi}{2} \right\} \tag{34}$$

and satisfies an estimate

$$\| p^2 u \| \leq c(\| \mathrm{H}(\mathrm{X}, \lambda) u \| + \| u \|) \tag{35}$$

for all $u \in \mathrm{D}(p^2)$, *where* a, b, c *are positive numbers depending on* ε *but not on* λ. *Moreover,* $\lambda \to \mathrm{H}(\mathrm{X}, \lambda)$ *is an analytic family of type* A *in the disc* $|\lambda| < 2^{-\frac{1}{2}}$.

Remark. — m-sectorial means that the numerical range *and* the spectrum of $\mathrm{H}(\mathrm{X}, \lambda)$ are contained in S.

Proof. — The kinetic energy (17) has the form $\mathrm{T}_0(x, p)$ + lower order terms in p, with a leading term

$$\mathrm{T}_0(x, p) = p_i \mathrm{A}^{ik}(x) p_k, \tag{36}$$

where $\mathrm{A}^{ik} = \mathrm{J}^{im}\mathrm{J}^{km}$. In matrix notation: $\mathrm{A} = \mathrm{B}^{-1}$, $\mathrm{B} = \mathrm{J}^{\mathrm{T}}\mathrm{J}$, $\mathrm{J} = 1 + \lambda \mathrm{V}$, $\mathrm{V} = (v_{i,k})$. First we estimate the quadratic form $(\xi, \mathrm{B}\xi)$ on C^3 for $|\xi| = 1$. Since V is real we have $\mathrm{V}^{\mathrm{T}} = \mathrm{V}^*$ and

$$(\xi, \mathrm{B}\xi) = 1 + 2\lambda \operatorname{Re}(\xi, \mathrm{V}\xi) + \lambda^2(\mathrm{V}\xi, \mathrm{V}\xi) = 1 + 2\lambda\eta r + \lambda^2 r^2,$$

where $r = |\mathrm{V}\xi| \leq 1$ by (30), and with real η in $-1 \leq \eta \leq +1$. Therefore $(\xi, \mathrm{B}\xi)$ lies on the straight line between the two complex numbers $(1 \pm \lambda r)^2$. It follows from (33) that $(\xi, \mathrm{B}\xi)$ is in a sector

$$\mathrm{S}_0 = \left\{ z \,|\, |\arg z| \leq b < \frac{\pi}{2} \right\} \tag{37}$$

with b depending only on ε. Since $b < \dfrac{\pi}{2}$ and $|1 \pm \lambda r| \geq 1 - 2^{-\frac{1}{2}} > 0$ we also have $\operatorname{Re}(\xi, \mathrm{B}\xi) \geq \delta(\varepsilon) > 0$. These properties carry over to $\mathrm{A} = \mathrm{B}^{-1}$, i. e.:

$$(\xi, \mathrm{A}\xi) \in \mathrm{S}_0, \qquad \operatorname{Re}(\xi, \mathrm{A}\xi) \geq \delta(\xi, \xi)$$

for some $\delta(\varepsilon) > 0$ and all $\xi \in \mathrm{C}^3$. For the leading term $\mathrm{T}_0(x, p)$ on $\mathrm{L}^2(\mathrm{R}^3)$ we thus obtain

$$(u, \mathrm{T}_0 u) \in \mathrm{S}_0; \qquad \operatorname{Re}(u, \mathrm{T}_0 u) \geq \delta(u, p^2 u), \tag{38}$$

for all $u \in \mathrm{D}(p^2)$. This extends directly to the leading term

$$\mathrm{T}_0 = \sum_{i=1}^{n} \mathrm{T}_0(x_i, p_i) \tag{39}$$

of the n-particle kinetic energy on $\mathrm{L}^2(\mathrm{R}^{3n})$. Next we prove that p^2 is bounded relative to T_0 in operator sense. By (38) we have

$$\begin{aligned} \| p^2 u \|^2 &= \sum_k (p_k u, p^2 p_k u) \leq \text{const.} \sum_k |(p_k u, \mathrm{T}_0 p_k u)| \\ &\leq \text{const.} \sum_k (|p_k^2 u, \mathrm{T}_0 u) + |(p_k u, [\mathrm{T}_0, p_k] u)|). \end{aligned} \tag{40}$$

In the first term we use that

$$|(p_k^2 u, T_0 u)| \leq \| p_k^2 u \| \, \| T_0 u \| \leq \delta \| p_k^2 u \|^2 + \delta^{-1} \| T_0 u \|^2 \tag{41}$$

for any $\delta > 0$. In the second term $[T_0, p_k]$ is of second order in p so that

$$\| [T_0, p_k] u \| \leq \text{const.} \| p^2 u \|$$

and therefore

$$\begin{aligned} |(p_k u, [T_0, p_k] u)| &\leq \delta \| p^2 u \|^2 + \text{const.}\, \delta^{-1} \| p_k u \|^2 \\ &\leq \delta \| p^2 u \|^2 + \text{const.}\, \delta^{-1} |(u, T_0 u)| \end{aligned} \tag{42}$$

for any $\delta > 0$. Inserting (41) (42) in (40), collecting all terms $\sim \| p^2 u \|^2$ on the left and choosing δ sufficiently small we arrive at

$$\| p^2 u \|^2 \leq \text{const.} (\| T_0 u \| \, \| u \| + T_0 u \|^2)$$

or

$$\| p^2 u \| \leq \text{const.} (\| T_0 u \| + \| u \|). \tag{43}$$

Inspection of this derivation shows that the constant in (43) depends only on ε and on bounds on the first and second derivatives of $v(x)$, but not on λ. Now we show that T_0 is m-sectorial with sector S_0. Let

$$A(\mu) = \mu T_0 + (1 - \mu) p^2, \qquad 0 \leq \mu \leq 1.$$

$A(\mu)$ is sectorial with sector S_0 and satisfies $\operatorname{Re}(u, A(\mu) u) \geq \delta (u, p^2 u)$ for some $\delta > 0$ independent of μ. As in the proof of (43) we derive that

$$\| p^2 u \| \leq \text{const.} (\| A(\mu) u \| + \| u \|)$$

with a constant independent of μ. Therefore

$$\| (A(\mu_1) - A(\mu_2)) u \| \leq \text{const.} | \mu_1 - \mu_2 | \, \| p^2 u \| \leq c | \mu_1 - \mu_2 | (\| (A(\mu_1) u \| + \| u \|)$$

with c independent of μ_1, μ_2. Suppose that $A(\mu_1)$ is m-sectorial. If $| \mu_1 - \mu_2 | < (2c)^{-1}$, $A(\mu_1) - A(\mu_2)$ has relative bound $< \frac{1}{2}$ with respect to $A(\mu_1)$, so that $A(\mu_2)$ is also m-sectorial by a standard argument. Since $A(0) = p^2$ is m-sectorial, we derive by a finite number of steps that $A(1) = T_0$ is m-sectorial.

Next we remark that $H(X, \lambda)$ is of the form $H(X, \lambda) = T_0 + R$ where the remainder R consists of first order terms in p and of potentials satisfying (29). Therefore R has arbitrarily small relative bound with respect to p^2. It follows from (43) that

$$\| Ru \| \leq \alpha \| T_0 u \| + \beta(\alpha) \| u \|$$

for any $\alpha > 0$ and uniformly in λ. We conclude that $H(X, \lambda) = T_0 + R$ is m-sectorial with a sector S of type (34) and that T_0 is bounded relative to $H(X, \lambda)$. The estimate (35) then follows from (43). Since for $|\lambda| < 2^{-\frac{1}{2}} H(X, \lambda)$

is m-sectorial with sector S and has constant domain $D(p^2)$, and since $H(X, \lambda)u$ is analytic in $|\lambda| < 1$ for all $u \in D(p^2)$, $H(X; \lambda)$ is an analytic family of type A for $|\lambda| < 2^{-\frac{1}{2}}$. ■

6. ANALYTIC VECTORS

Since the maps (27) and the corresponding unitary transformations $U(\lambda)$ do not form a group, we have to construct by hand a sufficiently large set A of « analytic vectors » ψ, for which $\lambda \to U(\lambda)\psi$ is analytic in some disc around $\lambda = 0$.

DEFINITION. — Let F be the algebra of entire functions $f(z)$ of $z = (z_1, \ldots, z_n)$; $z_i \in C^3$; with the following property: in any region

$$|\operatorname{Im} z| \leq (1 - \varepsilon)|\operatorname{Re} z| \qquad (\varepsilon > 0). \tag{44}$$

$f(z)$ vanishes faster than any inverse power of $|\operatorname{Re} z|$ as $|\operatorname{Re} z| \to \infty$. Here $|\ |$ stands for the norm in R^{3n}. We say that $\psi \in L^2(R^{3n})$ is an analytic vector if $\psi(x) = f(x)$ for some (unique) $f \in F$ and all $x \in R^{3n}$. The set of analytic vectors is denoted by A.

Evidently A is a linear subset of $L^2(R^{3n})$. Examples of functions $f \in F$ are

$$f(z) = e^{-\alpha z^2} P(z)$$

with $\alpha > 0$, $z^2 = z_1^2 + \ldots + z_n^2$ and P an arbitrary polynomial. This shows that A is dense in $L^2(R^{3n})$. For $\psi \in A$ we can define $U(\lambda)\psi$ for complex λ by

$$(U(\lambda)\psi)(x_1, \ldots, x_n) = J^{\frac{1}{2}}(x_1, \lambda) \ldots J^{\frac{1}{2}}(x_n, \lambda) f(x_1 + \lambda v(x_1), \ldots, x_n + \lambda v(x_n)) \tag{45}$$

where $f \in F$ is the entire function which reduces to ψ in R^{3n}. This definition is possible for $|\lambda| < 1$ by (32).

THEOREM 3. — *Let $v(x)$ be a vector field $R^3 \to R^3$ satisfying (6). Then we have:*

i) *For any $\psi \in A$, $\lambda \to U(\lambda)\psi$ is an L^2-valued analytic function in the disc $|\lambda| < 2^{-\frac{1}{2}}$;*

ii) *For any λ in this disc the image of A under $U(\lambda)$ is dense in $L^2(R^{3n})$.*

Proof. — For notational convenience we set $n = 1$. (6) implies $|v(x)| \leq v(0)| + |x|$, but since only the growth for $|x| \to \infty$ is relevant here, we will use the simpler bound

$$|v(x)| \leq |x|. \tag{46}$$

To prove *i*) we set $z(x) = x + \lambda v(x)$. Then

$$|\operatorname{Re} z|^2 - |\operatorname{Im} z|^2 \geq \frac{1}{2}|x|^2 - |\lambda|^2 |v|^2.$$

By (46) we then have for $|\lambda|^2 \leq \frac{1}{2} - \varepsilon$

$$|\operatorname{Re} z|^2 - |\operatorname{Im} z|^2 \geq \varepsilon |x|^2 \geq \varepsilon |v|^2 \geq 2\varepsilon |\operatorname{Im} z|^2. \tag{47}$$

Therefore $|\operatorname{Im} z| \leq (1+2\varepsilon)^{-\frac{1}{2}} |\operatorname{Re} z|$. On the other hand $|\operatorname{Re} z| \geq (1-2^{-\frac{1}{2}})|x|$, so that by (44) $(U(\lambda)\psi)(x)$ decreases faster than any inverse power of $|x|$ as $|x| \to \infty$, uniformly in λ for $|\lambda|^2 < \frac{1}{2} - \varepsilon$. Given this estimate, *i*) follows by remarking that $(\phi, U(\lambda)\psi)$ is analytic in $|\lambda| < 2^{-\frac{1}{2}}$ for any $\psi \in L^2(R^3)$.

To prove *ii*) we first note that $J^{\frac{1}{2}}(x, \lambda)$ and $J^{-\frac{1}{2}}(x, \lambda)$ are uniformly bounded by (32) for $|\lambda| \leq 2^{-\frac{1}{2}}$. Therefore we need only show that the functions

$$g(x) = f(x + \lambda v(x)); \qquad f \in F$$

are dense in $L^2(R^3)$. Given $h \in C_0^\infty(R^3)$ we construct a sequence $f_n \in F$ such that

$$g_n(x) = f_n(x + \lambda v(x)) \to h(x) \tag{48}$$

in L^2-norm as $n \to \infty$, namely

$$f_n(z) = \left(\frac{n}{\pi}\right)^{\frac{3}{2}} \int_{R^3} d^3y J(y, \lambda) h(y) \exp\left[-n(z-y-\lambda v(y))^2\right]. \tag{49}$$

Since h has compact support, $f_n(z)$ is an entire function with the same fall-off as $\exp(-nz^2)$, i. e. $f_n \in F$. To prove (48) we set $\xi = x-y+\lambda v(x)-\lambda v(y)$. From (6) it follows as in the case (47) that

$$|\operatorname{Re} \xi|^2 - |\operatorname{Im} \xi|^2 \geq \varepsilon |x - y|^2,$$

so that

$$|\exp(-\xi^2)| \leq \exp(-\varepsilon |x - y|^2). \tag{50}$$

Therefore

$$\left(\frac{n}{\pi}\right)^{\frac{3}{2}} \int_{R^3} d^3y J(y, \lambda) \exp\left[-n(x-y+\lambda v(x)-\lambda v(y))^2\right] = 1 \tag{51}$$

for all λ in the disc $|\lambda| < 2^{-\frac{1}{2}}$, since this integral is analytic in λ and equal to 1 for real λ by the transformation $y \to y + \lambda v(y)$ of the integration variable. It follows from (49) (50) (51) that

$$\begin{aligned} |h(x) - g_n(x)| &= \left| \left(\frac{n}{\pi}\right)^{\frac{3}{2}} \int d^3y J(y, \lambda)(h(x) - h(y)) \exp(-n\xi^2) \right| \\ &\leq \text{const. } n^{-\frac{3}{2}} \int d^3y \, |h(x)-h(y)| \exp(-n \in |x-y|^2), \end{aligned}$$

which vanishes in L^2-norm as a function of x as $n \to \infty$. ■

7. RESONANCES

Since X is fixed throughout this section we set $H(X) = H$ and $H(X, \lambda) = H(\lambda)$. As in the case of atoms, the spectrum of $H(\lambda)$ can best the understood by

inserting the electrons one by one into the given nuclear field. To describe this we will write $H^n(\lambda)$ whenever we want to exhibit the number n of electrons.

The essential spectrum of the differential operator $H^n(\lambda)$ depends only on its behavior outside any finite region of R^{3n}. To control this we now impose the condition (8) on the vector field $v(x)$. The following characterization of the spectrum of $H(\lambda)$ is the analogue of the Balslev-Combes theorem [2]:

THEOREM 4. — *Let $v(x)$ be any C^∞-vector field $R^3 \to R^3$ satisfying (6) (7) (8) and suppose that $|\lambda| < 2^{-\frac{1}{2}} - \varepsilon$ $(\varepsilon > 0)$. Then*

i) *$\sigma(H(\lambda))$ is independent of the choice of $v(x)$.*

ii)
$$\sigma_{ess}(H^n(\lambda)) = \sigma(H^{n-1}(\lambda)) + \sigma_0(\lambda) \tag{52}$$

for $n \geq 1$, where $\sigma(H^0(\lambda)) \equiv \{0\}$ and

$$\sigma_0(\lambda) = \{ z \mid \arg z = -2 \arg(1+\lambda) \}. \tag{53}$$

In particular, the complement $G(\lambda)$ of $\sigma_{ess}(H(\lambda))$ is simply connected and contains the complement G of the sector (34).

iii) *For any $\phi, \psi \in A$ and all $z \in G$ we have*

$$(\phi, (z - H)^{-1}\psi) = (U(\bar{\lambda})\phi, (z - H(\lambda))^{-1} U(\lambda)\psi). \tag{54}$$

Therefore $(\phi, (z - H)^{-1}\psi)$ has a meromorphic continuation in z from G to $G(\lambda)$ which we denote by the symbol $(\phi, (z - H)^{-1}\psi)_{G(\lambda)}$.

iv)
$$\sigma_{disc}(H(\lambda)) = \cup_{\phi,\psi \in A} \{ \textit{poles of } (\phi, (z - H)^{-1}\psi)_{G(\lambda)} \}. \tag{55}$$

v) *Let R be a discrete eigenvalue of $H(\lambda)$. If λ changes continuously, R remains a discrete eigenvalue of $H(\lambda)$ as long as $R \in G(\lambda)$.*

DISCUSSION. — By induction in n we obtain from this theorem the following familiar picture of $\sigma(H(\lambda))$, drawn for $\operatorname{Im} \lambda > 0$:

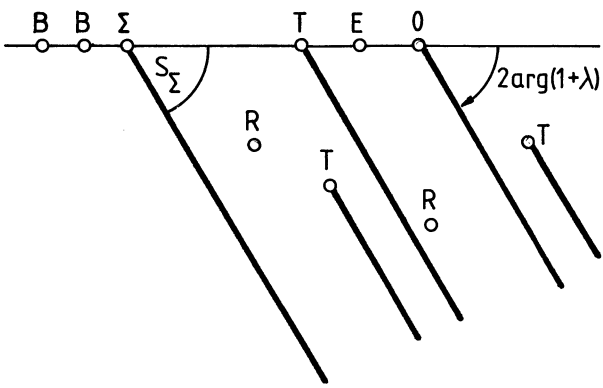

FIG. 1.

The essential spectrum of $H^n(\lambda)$ is given by

$$\sigma_{ess}(H^n(\lambda)) = T^n(\lambda) + \sigma_0(\lambda),$$

where

$$T^n(\lambda) = \bigcup_{m=0}^{n-1} \sigma_{disc}(H^m(\lambda))$$

is the « threshold set » of $H^n(\lambda)$ which always contains $\sigma_{disc}(H^0(\lambda)) \equiv \{0\}$. The leftmost threshold Σ is real and independent of λ. As $\arg(1+\lambda)$ decreases to zero, the ray $\Sigma + \sigma_0(\lambda)$ sweeps the sector S_Σ and becomes the essential spectrum $[\Sigma, \infty)$ of H. Eigenvalues B of $H(\lambda)$ outside S_Σ remain unchanged in this process, hence they are the (real) discrete eigenvalues of H. All other discrete eigenvalues E, R and thresholds T of $H(\lambda)$ belong to S_Σ. As $\arg(1+\lambda)$ decreases they remain fixed until they are covered by one of the rotating rays. Conversely, new eigenvalues and thresholds may be uncovered by the rotating parts of the essential spectrum. Discrete eigenvalues (and therefore thresholds) can accumulate only at thresholds, since any other accumulation point could be separated from $\sigma_{ess}(H(\lambda))$ by a small variation of $\arg(1+\lambda)$. As in the dilation-analytic case it can be shown that real discrete eigenvalues $E > \Sigma$ of $H(\lambda)$ survive at $\arg(1+\lambda) = 0$: they are the embedded, non-threshold eigenvalues of H [*2*]. We believe that $E < 0$ as in other n-body systems [*6*].

By definition, R is called a resonance if it is a non-real, discrete eigenvalue of $H(\lambda)$ for some λ in $|\lambda| < 2^{-\frac{1}{2}}$. By Theorem 4 the resonances are thus characterized by the pair (H, A) as the complex poles of the meromorphic continuation in z of all resolvent matrix elements $(\phi, (z-H)^{-1}\psi)$; $\phi, \psi \in A$; to a Riemann surface which is also determined by (H, A).

Proof of Theorem 4. — We proceed by induction in n, assuming that the theorem holds for $H^m(\lambda)$ if $m < n$. (The case $m = 0$ is trivial).

a) *Essential spectrum:* (52) is easily proved by « geometric spectral analysis » as described in [*5*]. We indicate the main steps. For a given configuration $(x_1 \ldots x_n) \in R^{3n}$ either $|x_i| < R$ $(i = 1 \ldots n)$ or the set $\{x_0 \equiv 0, x_1 \ldots x_n\} \subset R^3$ has diameter $\geq R$. In the second case there is a decomposition

$$D = (C_0, C_1); \qquad 0 \in C_0; \qquad C_1 \neq \emptyset \tag{56}$$

of the set $\{0 \ldots n\}$ into two clusters C_0, C_1 such that $|x_i - x_k| \geq R/n$ if $i \in C_0$ and $k \in C_1$. Hence there exists a smooth partition of unity

$$1 = \chi_0(x) + \sum_D \chi_D(x)$$

on R^{3n}, where D runs through all decompositions (56) and with the support properties

$$|x_i| \leq 2R \qquad \text{on supp } \chi_0 \text{ for all } i$$
$$|x_i - x_k| \geq R/n \qquad \text{on supp } \chi_D \text{ if } i \in C_0 \text{ and } k \in C_1 .$$

This means that on supp χ_D the electrons in the cluster C_1 are separated from the origin and from the other electrons by a distance $\geq R/n$. Taking R sufficiently large we thus have $v(x_i) = x_i$ by (8) for all $i \in C_1$. Then $H^n(\lambda)$ reduces in this region to

$$H_D^n(\lambda) = H^m(\lambda) \otimes 1 + 1 \otimes H_0^{n-m}(\lambda) \tag{57}$$

up to an error of order R^{-1} ($R \to \infty$), where $m < n$ is the number of electrons in C_0 and where

$$H_0^{n-m}(\lambda) = (1+\lambda)^{-2} \sum_{i \in C_1} p_i^2 + (1+\lambda)^{-1} \sum_{\substack{i,k \in C_1 \\ i<k}} |x_i - x_k|^{-1} \tag{58}$$

is the Hamiltonian of $n - m$ electrons without nuclear field, distorted by the simple scaling $x \to (1 + \lambda)x$. This operator is known to have the spectrum $\sigma_0(\lambda)$, because the electron-electron interaction is repulsive [*10*, section XIII.13, Example 5]. All the operators involved in (57) are sectorial by Theorem 2. Therefore it follows from (57) and Ichinose's lemma [*10*] that

$$\sigma(H_D^n(\lambda)) = \sigma(H^m(\lambda)) + \sigma_0(\lambda) . \tag{59}$$

By the induction hypothesis, $\sigma(H_D^n(\lambda))$ has no interior points. Based on the estimate (35) we can thus apply Theorem 3.3 of [*5*] which gives

$$\sigma_{ess}(H^n(\lambda)) = \bigcup_D \sigma(H_D^n(\lambda)) = \bigcup_{m=0}^{n-1} \sigma(H^m(\lambda)) + \sigma_0(\lambda) = \sigma(H^{n-1}(\lambda)) + \sigma_0(\lambda)$$

since $\sigma(H^m(\lambda)) \subset \sigma(H^{n-1}(\lambda))$ for $m < n$ by the induction hypothesis. This proves (*ii*). It follows from the induction hypothesis that $\sigma_{ess}(H^n(\lambda))$ is independent of the choice of $v(x)$ and has the form depicted in Fig. 1. Consequently, $G(\lambda) \equiv C \backslash \sigma_{ess}(H^n(\lambda))$ is simply connected and contains the complement G of the sector (34).

b) *Discrete spectrum:* Let $z \in G$. By Theorem 2, G is in the resolvent set of $H(\lambda)$ for $|\lambda| \leq 2^{-\frac{1}{2}} - \varepsilon$. For real λ in this disc (54) follows directly from (9) for arbitrary ϕ, ψ. Now let $\phi, \psi \in A$. By Theorems 2 and 3, (54) then extends by analytic continuation in λ to the disc $|\lambda| < 2^{-\frac{1}{2}} - \varepsilon$. This proves *iii*).

By (54) it is clear that poles of $(\phi_1(z - H)^{-1}\psi)_{G(\lambda)}$ can occur only at the discrete eigenvalues of $H(\lambda)$. Conversely, let $R \in \sigma_{disc}(H(\lambda))$ and let P be the corresponding spectral projection (i. e. the first order residue of

$(z - H(\lambda))^{-1}$ at the pole $z = R$). By Theorem 3 we can choose ϕ, $\psi \in A$ such that $(U(\bar{\lambda})\phi, PU(\lambda)\psi) \neq 0$. It then follows from (54) that R is a pole of $(\phi_1(z - H)^{-1}\psi)_{G(\lambda)}$. This proves *iv*), which in turn shows that $\sigma_{disc}(H(\lambda))$ and therefore the entire spectrum $\sigma(H(\lambda))$ is independent of the choice of $v(x)$.

To prove *v*), suppose that $R \in \sigma_{disc}(H(\lambda_0))$ and that

$$R \in \bigcap_{|\lambda - \lambda_0| < \varepsilon} G(\lambda) \equiv T.$$

By the induction hypothesis and by part (*a*) of the proof, T is open, simply connected and contains G (It is the complement of the sawtooth-shaped set which is swept by $\sigma_{ess}(H(\lambda))$ as λ runs through the disc $|\lambda - \lambda_0| < \varepsilon$). Thus R is a pole of $(\phi_1(z - H)^{-1}\psi)_T$ for some $\phi_1\psi \in A$ and therefore by *iv*) a discrete eigenvalue of $H(\lambda)$ for all λ in $|\lambda - \lambda_0| < \varepsilon$. ■

8. RESONANCE CURVES

In this section λ is fixed in $|\lambda| < 2^{-\frac{1}{2}}$. We set $H(X, \lambda) \equiv H(X)$ to exhibit only the dependence on the nuclear configuration X, which is restricted to some ball

$$|X - X^0| < d \tag{60}$$

of R^{3N}. Let $v(x)$ be a C^∞-vector field $R^3 \to R^3$ satisfying (6) and

$$v(x) = 0 \quad \text{if} \quad |x - X_r^0| < d \text{ for some } r. \tag{61}$$

Then (7) holds for all X in the ball (60) and we can use the same vector field to define H(X) in this ball. Consequently, $H(X) - H(X^0)$ consists only of terms arising from the nuclear potentials, and we have

$$\lim_{X \to X^0} \| (H(X) - H(X^0))(1 + p^2)^{-1} \| = 0. \tag{62}$$

This follows if

$$\lim_{y \to y_0} \| V(x, y) - V(x, y_0))(1 + p^2)^{-1} \| = 0 \tag{63}$$

on the one-electron Hilbert space $L^2(R^3)$, where $V(x, y)$ is given by (28). As a first step to prove (63) we approximate $V(x, y)$ by a smooth potential $V_\varepsilon(x, y)$, obtained from (28) by the regularisation

$$|x - y|^{-1} \to (|x - y| + \varepsilon)^{-1}$$

of the last factor. We remark that

$$\lim_{\varepsilon \to 0} \| (|x - y|^{-1} - (|x - y| + \varepsilon)^{-1})(1 + p^2)^{-1} \| = 0 \tag{64}$$

uniformly in y, since this norm is independent of y and since in

$$\left(\frac{|x|}{|x| + \varepsilon}\right)\left(\frac{1}{|x|}(1 + p^2)^{-1}\right)$$

the first factor converges strongly to 1 while the second is compact. By (64) $V_\varepsilon(x, y)(1 + p^2)^{-1}$ approximates $V(x, y)(1 + p^2)^{-1}$ in norm as $\varepsilon \to 0$, uniformly in y. Therefore we need only prove (63) for the regularised potential, which is straightforward. As a consequence of (62) and (35) we have:

THEOREM 5. — *Let $v(x)$ ba a C^∞-vector field $R^3 \to R^3$ satisfying (6), which vanishes in a neighbourhood of each point $X_1^0 \ldots X_N^0$. Then $H(X) \to H(X^0)$ in norm-resolvent sense as $X \to X^0$: if $z \in \rho(H(X^0))$, then $z \in \rho(H(X))$ for X close to X^0 and*

$$\lim_{X \to X^0} \| (z - H(X))^{-1} - (z - H(X^0))^{-1} \| = 0 .$$

Therefore each discrete eigenvalue of $H(X^0)$ is stable [8] with respect to the family $H(X)$.

Less precisely this can be summarized by saying that the resonances depend continuously on the nuclear coordinates, or that « resonance curves are continuous ». Analyticity in X derives from the following analogue of Theorem 1:

THEOREM 6. — *In addition to the hypothesis of Theorem 5 we assume that*

$$X_r^0 \neq X_s^0 \qquad \text{if} \qquad r \neq s . \tag{65}$$

For small $\xi \in R^{3N}$ we then have

$$H(X^0 + \xi) = U(\xi)^{-1} \tilde{H}(\xi) U(\xi),$$

where $U(\xi)$ is unitrary and where $\tilde{H}(\xi)$ is an analytic family of type A for small $\xi \in C^{3N}$.

Proof. — By hypothesis, $v(x)$ satisfies (61) for some $d > 0$. Therefore we can choose real C^∞-functions $f_r(x)$ with support in $| x - X_r^0 | < d/2$ and with $f_r(X_s^0) = \delta_{rs}$ $(r, s = 1 \ldots N)$. Let

$$w(x) = \sum_r \xi_r f_r(x) .$$

By construction, $v(x + w(x)) = v(x)$ for small $\xi = (\xi_1 \ldots \xi_N) \in R^{3N}$ and all x. Let $U(\xi)$ be the unitrary operator (16) corresponding to the map $x \to x + w(x)$ for small $\xi \in R^{3N}$. Then

$$\tilde{H}(\xi) \equiv U(\xi) H(X^0 + \xi) U(\xi)^{-1}$$

is the Hamiltonian distorted by the composite map

$$x \to x + w(x) + \lambda v(x + w(x)) = x + \lambda v(x) + w(x) . \tag{66}$$

Explicitely, $\tilde{H}(\xi)$ is given by (26) if $J_{ik}(x)$ is taken as the Jacobian of the map (66) and if $v(x)$ is replaced in (24) (25) by $\lambda v(x) + w(x)$. It then follows

as in the proof of Theorem 1 that $\tilde{H}(\xi)$ is an analytic family of type A for small $\xi \in C^{3N}$. ■

By this theorem we can apply analytic perturbation theory to study the local behaviour of resonance curves. In particular, non-degenerate resonances are analytic in $X \in C^{3N}$ in a neighbourhood of any nuclear configuration X^0 satisfying (65).

Note added in proof. — Time evolution for electrons in the field of classical moving nuclei.

In this note we discuss existence and uniqueness of solutions to

$$i\dot{\psi} \equiv i\frac{d\psi}{dt} = H(t)\psi(t), \tag{67}$$

where $H(t) \equiv H(X(t))$ is given by (1) in terms of a prescribed motion $X(t)$ of the nuclei. Here again it is the lack of smoothness of $H(t)$ in t (due to the moving Coulomb singularities) which prevents a straightforward application of standard existence and uniqueness theorems.

In a recent paper, Wüller [*14*] has given a partial solution of this problem: his analysis is restricted to nuclear configurations of the type

$$X_r(t) = l(t)R(t)X_r(0); \qquad r = 1 \ldots N,$$

where $l(t) > 0$ and where $R(t)$ is a rotation in some fixed plane. More recently, Yajima [*15*] has proven a powerful general existence and uniqueness theorem for solutions of (67) with Hamiltonians of the form

$$H(t) = -\Delta + V(t, x) \quad \text{on} \quad R^m,$$

which easily accommodates the moving Coulomb singularities in our problem. This result completely answers the question raised above. The point we wish to make is that a time dependent distortion transforms (67) into an evolution equation with smooth generator. It appears that repulsive moving singularities of arbitrary strength (and moving walls) can be handled in the same spirit. We illustrate the method by proving:

THEOREM 7. — *Let $t \to X(t)$ be a C^2-function from R to R^{3N} satisfying*

$$X_r(t) \neq X_s(t)$$

for $r \neq s$ and all t. Then (67) has a unique global strong solution $t \to \psi(t) \in D(p^2)$ for any initial state $\psi(t_0) \in D(p^2)$.

Proof. — Given any initial time t_0 we prove existence and uniqueness of solutions in an open time interval $|t - t_0| < T$. As in (22) we construct a vector field

$$v(x, t) = \sum_{r=1}^{N} \xi_r(t) f_r(x) \tag{68}$$

with

$$\xi(t) = X(t) - X(t_0)$$

and real C_0^∞-functions $f_1 \ldots f_N$ on R^3 satisfying

$$f_r(X_s(t_0)) = \delta_{rs}.$$

For sufficiently small T we have

$$\| v_{i,k}(x, t) \| < \frac{1}{2}$$

for all x and $| t - t_0 | < T$. The unitary operator (16) for this vector field is then well defined and depends on t: we denote it by $U(t)$. The transformed Hamiltonian

$$\tilde{H}(t) \equiv U(t)H(t)U(t)^{-1}$$

is given explicitely by (26) with $X_r \equiv X_r(t_0)$; i. e. the moving Coulomb singularities are transformed to rest. Defining

$$\varphi(t) = U(t)\psi(t),$$

(67) transformes into

$$i\dot{\varphi} = [\tilde{H}(t) + D(t)]\varphi(t) \equiv A(t)\varphi(t) \tag{69}$$

with

$$D(t) = i\dot{U}(t)U(t)^{-1}.$$

This is readily evaluated in explicit symmetric form: $D(t)$ is the sum of the one-electron operators

$$D(t) = \frac{1}{2}(\dot{v}_k U p_k U^{-1} + U p_k U^{-1} \dot{v}_k)$$

$$= \frac{1}{2}(\dot{v}_k J^{\frac{1}{2}} J^{mk} p_m J^{-\frac{1}{2}} + J^{-\frac{1}{2}} p_m J^{mk} J^{\frac{1}{2}} \dot{v}_k),$$

where

$$\dot{v}(x, t) = \sum_{r=1}^{N} \dot{\xi}_r(t) f_r(x).$$

The structure of the generator $A(t)$ is now apparent. Its kinetic part is a sum of one-particle operators

$$p^2 + a_{ik}(x, t)p_i p_k + a_i(x, t)p_i + a(x, t)$$

on $L^2(R^3)$, where the a's are bounded multiplication operators which vanish in norm as $t \to t_0$ and which are as smooth in t as $\dot{X}(t)$. The potential part is a sum of time independent Coulomb potentials

$$| x_i - x_k |^{-1}; \qquad | x_i - X_r(t_0) |^{-1}.$$

multiplied by time dependent bounded functions which (in sup norm) are as smooth in t as $X(t)$. Since $X(t)$ is C^2, $A(t)$ is a C^1-function from

$|t - t_0| < T$ to the space of bounded operators from $D(p^2)$ to L^2 (differentiable in norm sense). Moreover, we can choose T sufficiently small to have

$$\| p^2\psi \| \leq \alpha \| A(t)\psi \| + \beta \| \psi \|$$

for all t in $|t - t_0| < T$. Therefore

$$B(t, s) = (i + A(t))(i + A(s))^{-1}$$

is norm-differentiable in t as a bounded operator on L^2. This is largely sufficient to apply e. g. Kato's theorem [*13*] [*16*], which states that (69) has a unique strong solution $\varphi(t) \in D(p^2)$ for any given initial value $\varphi(t_0) \in D(p^2)$. The corresponding result for (67) then follows by observing that $U(t)$ maps $D(p^2)$ onto itself. ■

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