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COMPLEX-POTENTIAL DESCRIPTION OF THE DAMPED HARMONIC OSCILLATOR.

I. The Propagator

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1. Introduction

There is a large number of problems ranging from elementary particles to statistical physics, in which the considered systems are dissipative (cf.,e.g., [1-5]). The dynamics in such cases can be rarely described fully, including interaction with the heat reservoir (decay products, compound nucleus channel,etc.), usually one is forced to express influence of these degrees of freedom by means of phenomenological Lagrangians or Hamiltonians. They can be constructed in different ways : as time-dependent, non-linear (e.g., [3,6]) or non-selfadjoint, in particular Hamiltonians with complex potentials are popular in practical calculations in nuclear physics.

Recently we have shown how to incorporate description of a dissipative system S via a phenomenological non-selfadjoint Hamiltonian H into the standard quantum-theoretical framework [7]. If H is closed and iH generates a continuous contractive semigroup (such operators we called pseudo-Hamiltonians), then by minimal unitary dilation of this semigroup we obtain objects which are naturally interpretable as the state Hilbert system of a larger isolated system Σ containing S and the unitary evolution group of Σ . The well-known difficulty with spectrum of the corresponding total Hamiltonian (see [4,8] and references therein) means that the semigroup evolution of S is necessarily approximative [7], however, this approximation is good enough for a lot of applications [9,10].

In the present paper, we apply the pseudo-Hamiltonian approach to the case of multidimensional harmonic oscillator with damping. There are, of course, many possibilities how to choose H ; some complex structures have been already studied [11]. We shall use the most natural choice $H = -\frac{1}{2}\Delta + x.(A-iW)x$, where A,W are strictly positive matrices (strict positivity of A is assumed for convenience, in fact, the proofs can be carried out for positive A as well). We assume neither a time-dependent frequency [6] , nor any driving force, stochastic or not [6,12]. On the other hand, we assume oscillators of an arbitrary dimension d ; the generalization to the $d>1$ case is non-trivial, because A, W need not be simultaneously diagonalizable. This multidimensionality together with the special choice of H could be of some interest for the old problem of constructing a field theory with basic quanta metastable.

One has to check first that our H is a pseudo-Hamiltonian in the sense of the above definition. If the damping part could be regarded as a perturbation to the undamped oscillator, the Kato-Rellich type lemma would be applicable. In general, however, this is not so. Thus we use a trick based on a successive application of the lemma ; this trick might appear to be useful for some self-adjointness proofs too.

The main result of the paper is an explicit integral-operator expression of the evolution semigroup corresponding to H . After some preliminaries, we prove it in Secs.5,6. The method is based on Feynman-type path integrals in the sense of Nelson, i.e., defined by Lie-Trotter formula [13,14]. The same result, however, is obtained with some other definitions of the path integral, for instance that one of Truman [15,16] or that using the "uniform" Trotter formula [17].

The obtained results will be discussed in the second part of this paper [18]. For the sake of simplicity, we shall limit ourselves there essentially to the one-dimensional case. The discussion will concern the problems of non-damped and classical limits, further we shall find the point spectrum of H .

2. Some notation and conventions

$Q^2 = \sum_{j=1}^{d} Q_j^2$, where $(Q_j\psi)(x) = x_j\psi(x)$,

$P^2 = \sum_{j=1}^{d} P_j^2 = -\Delta$, where $P_j = F_d^{-1}Q_jF_d$ and F_d is the d-dimensional Fourier-Plancherel operator,

$v_1(x) = x.Ax$, $v_2(x) = x.Wx$, where A , W are real positive $d \times d$ matrices (more exactly, positive symmetric operators on $\mathbb{R}^d$) and $v(x) = v_1(x) - iv_2(x) = x.Bx$,

V_i : $(V_i\psi)(x) = v_i(x)\psi(x)$, $V = V_1 - iV_2$,

$H_1 = \frac{1}{2} P^2 + V_1$,

$H_2 = H_1 \restriction \mathcal{S}(\mathbb{R}^d)$, $H_3 = H_2 - iV_2 = H \restriction \mathcal{S}(\mathbb{R}^d)$,

$H = H_1 - iV_2 = \frac{1}{2} P^2 + V$,

$\mathcal{M}(\mathcal{H})$ is the set of all (finite) complex Borel measures on a real separable Hilbert space $\mathcal{H}$,

$\mathcal{F}(\mathcal{H})$ is the set of functions f : $f(y) = \int_{\mathcal{H}} \exp(i(y,y'))\, d\mu(y')$, where $\mu \in \mathcal{M}(\mathcal{H})$ and $(.,.)$ is the inner product of $\mathcal{H}$.

In what follows, square roots of complex numbers and matrices will appear frequently. It is useful to make an overal choice of the branch : we prefer to work with $(e^{i\varphi})^{1/2} = \exp(\frac{1}{2} i\varphi)$, $0 \leq \varphi < 2\pi$. There is a particular case which should be mentioned : when complex frequencies are considered, it is more natural to have their real parts positive, at least from the viewpoint of non-damped limit. We shall use therefore $\Omega = -(2B)^{1/2}$ with the square root understood in the above sense.

3. The pseudo-Hamiltonian property of H

As mentioned above, throughout this section we assume the matrices A, W to be strictly positive (as operators on $\mathbb{R}^d$). The eigenvalues of A are α_j , $j = 1,\ldots,d$, so $\alpha \equiv \min_{1 \leq j \leq d} \alpha_j > 0$. The inequalities

$$\alpha^2 \|Q^2\psi\|^2 \leq \|V_1\psi\|^2 = \sum_{j,k=1}^{d} \alpha_j \alpha_k \|Q_j Q_k \psi\|^2 \leq \|A\|^2 \|Q^2\psi\|^2$$

show that $D(V_1) = D(Q^2)$, analogously $D(V_2) = D(Q^2)$, i.e.,

$$D(H) = D(H_1) = D(P^2) \cap D(Q^2) \quad . \qquad (1)$$

__Proposition 1__ : H_1 is self-adjoint.

Proof : We notice first that H_2 is e.s.a. due to existence of a complete set of eigenvectors $\subset \mathcal{S}(\mathbb{R}^d)$. Both P^2 and V_1 are self-adjoint and therefore closed so that $H_1 \subset \overline{H}_2$. In order to prove the opposite inclusion we shall verify that there is $b > 0$ such that

$$\frac{1}{4} \|P^2\psi\|^2 + \|V_1\psi\|^2 \leq \|H_2\psi\|^2 + b\|\psi\|^2 \quad , \quad \psi \in \mathcal{S}(\mathbb{R}^d) \quad . \tag{2}$$

We have $(P_j\psi)(x) = -i\partial\psi(x)/\partial x_j$ for these ψ , i.e.,

$$((P_jQ_k - Q_kP_j)\psi)(x) = -i\,\delta_{jk}\,\psi(x) \quad , \quad \psi \in \mathcal{S}(\mathbb{R}^d) \quad . \tag{3}$$

We choose a basis in $\mathbb{R}^d$ so that A is diagonal, then

$$(\psi,(P^2V_1 + V_1P^2)\psi) \geq \sum_{j=1}^{d} \alpha_j(\psi,(P_j^2Q_j^2 + Q_j^2P_j^2)\psi) \quad ,$$

because $(\psi, P_j^2Q_k^2\psi) \geq 0$ for $j \neq k$ due to the relations (3), which further imply

$$(\psi,(P^2V_1 + V_1P^2)\psi) \geq \frac{1}{2} \sum_{j=1}^{d} \alpha_j \|(P_j^2Q_j^2 + Q_j^2P_j^2)\psi\|^2 - \frac{3}{2}\|\psi\|^2 \operatorname{Tr} A \quad .$$

Thus (2) holds if $b \geq \frac{3}{4} \operatorname{Tr} A$. Assume now $\psi \in D(\overline{H}_2)$. If $\{\psi_n\}$ is a sequence $\subset \mathcal{S}(\mathbb{R}^d)$, $\psi_n \to \psi$, then $\{H_2\psi_n\}$ converges too, i.e., $\|H_2\psi_n - H_2\psi_m\| \to 0$ with $n,m \to \infty$. The inequality (2) shows that also $\{P^2\psi_n\}$ and $\{V_1\psi_n\}$ converge, however, both P^2, V_1 are closed and $\mathcal{S}(\mathbb{R}^d) \subset D(P^2) \cap D(V_1)$ so that $\psi \in D(P^2) \cap D(V_1) = D(H_1)$. ∎

The pseudo-Hamiltonian property of H will be proved below by successive applications of the following perturbative lemma (cf. [7]; [14], sec.X.8) :

Proposition 2 : Let G be a densely defined closable operator on a Hilbert space $\mathcal{H}$ such that $\overline{G}$ is a pseudo-Hamiltonian. Let further C be closed and accretive, $D(C) \supset D(G)$, and assume that there exist non-negative $a < 1$, b such that

$$\|C\psi\|^2 \leq a^2\|G\psi\|^2 + b^2\|\psi\|^2 \quad , \quad \psi \in D(G) \quad . \tag{4}$$

Then $D(\overline{G}) \subset D(C)$ and the operator $\overline{G} - iC$ defined on $D(\overline{G})$ is closed and belongs to the class of pseudo-Hamiltonians.

One must exhibit conditions under which (4) is fulfilled in the case under consideration :

Proposition 3 : (a) Let $b^2 \leq \frac{1}{2}\alpha\|W\|^{-1}$, then there is a positive c such that

$$\|bV_2\psi\|^2 \leq \frac{1}{2}\|H_1\psi\|^2 + c\|\psi\|^2 \quad , \quad \psi \in \mathcal{S}(\mathbb{R}^d) \quad . \tag{5a}$$

(b) Let $a > 0$ and $b^2 \leq \frac{1}{2}a^2$, then there is a positive c such that

$$\|bV_2\psi\|^2 \leq \frac{1}{2}\|(H_1 - iaV_2)\psi\|^2 + c\|\psi\|^2 \quad , \quad \psi \in \mathcal{S}(\mathbb{R}^d) \quad . \tag{5b}$$

Proof : We have to find c for which

$$I \equiv (\psi, (\tfrac{1}{2}(H_1 + iaV_2)(H_1 - iaV_2) - bV_2^2 + c)\psi)$$

is non-negative independently of $\psi \in \mathcal{S}(\mathbb{R}^d)$. We choose again a basis in $\mathbb{R}^d$ so that A is diagonal and denote by W_{jk} the corresponding matrix elements of W . Expressing $(V_2P^2 - P^2V_2)\psi$ and $(V_1P^2 + P^2V_1)\psi$ from (3) and omitting the positive term $\frac{1}{8}(\psi, P^4\psi)$, we obtain

$$I \geq (\psi, \Big[\frac{1}{8}\sum_{j=1}^{d}\alpha_j(P_kQ_j + Q_jP_k)^2 - \frac{3}{8}\operatorname{Tr}A + \frac{1}{2}\Big(\sum_{j=1}^{d}\alpha_jQ_j\Big)^2 +$$

$$+ (\tfrac{1}{2}a^2 - b^2)\Big(\sum_{j,k=1}^{d}W_{jk}Q_jQ_k\Big)^2 - \frac{a}{4}\sum_{j,k=1}^{d}W_{jk}(P_kQ_j + Q_jP_k) + c\Big]\psi) \quad .$$

Assume first $a = 0$ and $b^2 \leq \frac{1}{2}\alpha\|W\|^{-1}$, then the last inequality yields

$$I \geq (\psi, \Big[c - \frac{3}{8}\operatorname{Tr}A + (\tfrac{1}{2}\alpha - b^2\|W\|)Q^2\Big]\psi) \geq (c - \frac{3}{8}\operatorname{Tr}A)\|\psi\|^2$$

so that (5a) holds if $c \geq \frac{3}{8}\operatorname{Tr}A$. On the other hand, if $a^2 \geq 2b^2$, then

$$I \geq (\psi, \Big[\sum_{j,k=1}^{d}(8\alpha_j)^{-1}(\alpha_j(P_kQ_j + Q_jP_k) - aW_{jk})^2 -$$

$$- \frac{1}{8}a^2\sum_{j,k=1}^{d}\alpha_j^{-2}W_{jk}^2 + c - \frac{3}{8}\operatorname{Tr}A\Big]\psi) \quad ,$$

and therefore (5b) holds if $c \geq \frac{3}{8}\operatorname{Tr}A + \frac{1}{8}a^2\sum_{j,k=1}^{d}\alpha_j^{-2}W^2_{jk}$. ∎

Combining now the above three auxiliary statements, we can prove the main result of this section :

<u>Theorem 1</u> : Let A, W be strictly positive so that (1) holds, then H is closed and belongs to the class of pseudo-Hamiltonians. Moreover, $\mathcal{S}(R^d)$ is a core for H, i.e., $H = \overline{H}_3$.

<u>Proof</u> : (a) If $\alpha \geqslant 2\|W\|$, then there is $c > 0$ such that (5a) with $b = 1$ holds. The operator V_2 is positive, and therefore accretive, $D(V_2) \supset D(H_1)$ and $H_1 = \overline{H}_2$ is a pseudo-Hamiltonian due to Proposition 1. Applying then Proposition 2 to $G = H_2$, $C = V_2$ we see that for $H = H_1 - iV_2$ the assertion is valid.
(b) If $\alpha < 2\|W\|$ we choose k positive, $2\|W\|k^2 \leqslant \alpha$, and n natural so that

$$k(1 + 2^{-1/2})^{n-1} = 1 \quad . \qquad (*)$$

The same argument as above shows that the operator $H_1 - ikV_2$ with the domain $D(H_1)$ is closed and belongs to the pseudo-Hamiltonian class. Moreover, this operator equals $\overline{H_2 - ikV_2}$: obviously $\overline{H_2 - ikV_2} \subset H_1 - ikV_2$; on the other hand, for an arbitrary $\varphi \in D(H_1)$ and a sequence $\{\varphi_n\} \subset \mathcal{S}(R^d)$, $\varphi_n \to \varphi$, we have $(H_2 - ikV_2)\varphi_n = H_1\varphi_n - ikV_2\varphi_n$ so that $\varphi \in D(\overline{H_2 - ikV_2})$.
(c) The proof is completed by induction : assume that the assertion holds for $H_{1j} = \overline{H}_{2j}$, where $H_{sj} = H_s - ik(1+2^{-1/2})^{j-1}V_2$. The assumption of Proposition 3(b) is fulfilled for $a = 2^{1/2}b = k(1 + 2^{-1/2})^{j-1}$, thus (5b) together with Proposition 2 imply that the assertion holds for

$$H_{1j} - ik2^{-1/2}(1 + 2^{-1/2})^{j-1} = H_{1,j+1}$$

as well. In the same way as above one proves $H_{1,j+1} = \overline{H}_{2,j+1}$. Since the assertion is valid for $H_{11} = \overline{H}_{21}$ due to (b), the same is true for H_{1j} corresponding to any natural j, in particular for $H_{1n} = \overline{H}_{2n}$ which equals $H = \overline{H}_3$ in view of (*). ∎

4. An auxiliary integral formula

In the next section, the following integral will be useful

$$I_N(M,\ ) = \int_{\mathbb{R}^N} \exp\left\{ \frac{i}{2}\, \xi\cdot M\xi + i\,\xi\cdot\eta \right\} d\xi \quad , \tag{6}$$

where M is a symmetric $N\times N$ matrix the imaginary part of which is assumed strictly positive, $\mathrm{Im}\ \xi\cdot M\xi > 0$ for each non-zero $\xi\in\mathbb{R}^N$, and η is a complex vector, $\eta = \eta^{(1)} + i\,\eta^{(2)}$ with $\eta^{(i)}\in\mathbb{R}^N$.

The quadratic form $\xi\mapsto\xi\cdot M\xi$ can be "diagonalized", i.e., there exists S such that $M = S^T S$, further M is regular due to the assumption so the same is true for S. Completing now to the full square in the exponent, one obtains

$$I_N(M,\eta) = \exp\left\{-\frac{i}{2}\,\eta\cdot M^{-1}\eta\right\}\ J_N(M,\eta) \quad , \tag{7}$$

$$J_N(M,\eta) = \int_{\mathbb{R}^N} \exp\left\{ \frac{i}{2}\left[S(\xi + M^{-1}\eta)\right]^2\right\} d\xi \quad ; \tag{8}$$

the last integral can be easily seen to exist due to the assumed strict positivity of $\mathrm{Im}\, M$. Notice that in the case of real M, η the integrals (6),(8) exist in the improper sense only, but the evaluation of $J_N(M,\eta)$ is not complicated : (a) translational invariance of $d\xi$ implies its independence of η and (b) the substitution of $\xi' = S\xi$ into $J_N(M,0)$ gives

$$J_N(M,\eta) = (2\pi i)^{N/2}(\det M)^{-1/2} \quad . \tag{9}$$

None of these tricks is applicable in the case of complex M even if η is real. Nevertheless, the relation (9) remains valid as shown below :

<u>Proposition 4</u> : If M is symmetric with strictly positive imaginary part, then the integral (6) is given by (7)-(9).

In order to evaluate the integral (8), let us first verify that the η-independence is preserved in the complex case :

<u>Lemma 4.1</u> : $J_N(M,\eta) = J_N(M,0)$ for each $\eta\in\mathbb{C}^N$.

<u>Proof</u> : We introduce the function $K : \mathbb{C}^N\to\mathbb{C}$ by

$$K(\zeta) = J_N(M,M\zeta) - J_N(M,0) = \int_{\mathbb{R}^N} \exp\left\{\frac{i}{2}(S(\xi+\zeta))^2\right\} d\xi - J_N(M,0) \quad .$$

For each j, the function $h_j(\cdot) = K(\zeta_1,\dots,\zeta_{j-1},\cdot,\zeta_{j+1},\dots,\zeta_N)$

with $\zeta_1,\dots,\zeta_{j-1},\zeta_{j+1},\dots,\zeta_N$ fixed is holomorphic in $\mathbb{C}$,

$$h_j'(\zeta_j) = i \int_{\mathbb{R}^N} (M(\xi+\zeta))_j \exp \tfrac{1}{2}(S(\xi+\zeta))^2 \, d\xi \quad ,$$

and therefore K is holomorphic in $\mathbb{C}^N$ due to the basic theorem of Hartogs ([19] , § 2.II.2). Translational invariance of the Lebesgue measure implies $K(\zeta) = 0$ for all $\zeta \in \mathbb{R}^N$, then $K(\zeta) = 0$ for each $\zeta \in \mathbb{C}^N$ too ([19] , § 2.II.3). Since M is regular due to the assumption, the assertion follows. ∎

The rest of the proof consists of evaluating $J_N(M,0) = I_N(M,0)$. To this purpose, some recursive relations for minors of M are useful. Let us denote

$$\Delta(m,j) = \det \begin{pmatrix} M_{11} & M_{12} & & M_{1m} \\ \cdots & \cdots & \cdots & \cdots \\ M_{m-1,1} & M_{m-1,2} & \cdots & M_{m-1,m} \\ M_{j1} & M_{j2} & \cdots & M_{jm} \end{pmatrix} \tag{10}$$

for $j = m, m+1, \dots, N$, in particular, $\Delta_m \equiv \Delta(m,m)$ is the m-th principal minor of M .

<u>Lemma 4.2</u> : Let Δ_m , $m = 1,\dots,N$, be non-zero and set $\Delta_0 = 1$, then

$$M_{j,k+1} - \sum_{m=1}^{k} \frac{\Delta(m,j)\Delta(m,k+1)}{\Delta_{m-1}\,\Delta_m} = \frac{\Delta(k+1,j)}{\Delta_k} \tag{11}$$

holds for $j = k+1, k+2, \dots, N$.

<u>Proof</u> : Since M is symmetric matrix of rank N , it can be expressed as $M = BB^T$, where B is the following lower-triangular matrix (cf. [20] , § II.4) :

$$B_{jm} = (\Delta_{m-1}\Delta_m)^{-1/2}\,\Delta(m,j) \quad , \quad m = 1,\dots,N \, , \quad j = m, m+1, \dots, N \, .$$

Substituting into the lhs of (11), we obtain

$$M_{j,k+1} - \sum_{m=1}^{k} B_{jm}B_{k+1,m} = M_{j,k+1} - \sum_{m=1}^{k+1} B_{jm}(B^T)_{m,k+1} +$$

$$+ B_{j,k+1}B_{k+1,k+1} = \Delta(k+1,j)/\Delta_k \quad .$$ ∎

Now we are ready to prove that

$$I_N(M,0) = \int_{\mathbb{R}^N} \exp\left\{ \frac{i}{2} \sum_{j,l=1}^{N} M_{jl}\xi_j\xi_l \right\} d\xi_1 \dots d\xi_N \qquad (*)$$

is expressed by (9). This is true for $N = 1$ (cf. [21], 3.923), i.e., one has

$$\int_{\mathbb{R}} \exp\left\{ \frac{i}{2} c\xi^2 + ib\xi \right\} d\xi = \left(\frac{2\pi i}{c}\right)^{-1/2} \exp(-\frac{i}{2c} b^2) \qquad (**)$$

for $\operatorname{Im} c > 0$. If $N > 1$, we perform the integration in (*) successively using (**) : we integrate first, say, over ξ_1, then over ξ_2, etc. Let us assume that the k-th integration gives

$$I_N(M,0) = (2\pi i)^{k/2}(\Delta_k)^{-1/2} \int_{\mathbb{R}^{N-k}} d\xi_{k+1}\dots d\xi_N \exp\left\{\frac{i}{2} \sum_{j,l=k+1}^{N} M_{jl}\xi_j\xi_l - \right.$$

$$\left. - \frac{i}{2} \sum_{m=1}^{k} (\Delta_{m-1}\Delta_m)^{-1}\left(\sum_{j=k+1}^{N} \xi_j \Delta(m,j)\right)^2 \right\} . \qquad (***)$$

Now one has to separate terms in the exponent containing the second, first and zero power of ξ_{k+1} , and to integrate over it using (**) ; this leads to

$$I_N(M,0) = (2\pi i)^{(k+1)/2}\left[\Delta_k\left(M_{k+1,k+1} - \sum_{m=1}^{k} \frac{(\Delta(m,k+1))^2}{\Delta_{m-1}\Delta_m}\right)\right]^{-1/2} .$$

$$\cdot \int_{\mathbb{R}^{N-k-1}} d\xi_{k+2}\dots d\xi_N \exp\left\{ \frac{i}{2} \sum_{j,l=k+2}^{N} M_{jl}\xi_j\xi_l - \frac{i}{2} \sum_{m=1}^{k} (\Delta_{m-1}\Delta_m)^{-1} . \right.$$

$$\left. \cdot\left(\sum_{j=k+2}^{N} \xi_j \Delta(m,j)\right)^2 \right\} \exp\left\{ - \frac{i}{2}\left(M_{k+1,k+1} - \sum_{m=1}^{N} \frac{(\Delta(m,k+1))^2}{\Delta_{m-1}\Delta_m}\right)^{-1} . \right.$$

$$\left. \cdot \sum_{j=k+2}^{N} \xi_j\left(M_{j,k+1} - \sum_{m=1}^{k} \frac{\Delta(m,j)\Delta(m,k+1)}{\Delta_{m-1}\Delta_m}\right)^2 \right\} .$$

Since M is regular, its determinant is non-zero. Assume for a moment that the same is true for all principal minors, then the last expression simplifies by Lemma 4.2 and gives (***) with k replaced by $k+1$. Consequently, if (***) holds for $k = 0,1,\dots$ $\dots,k_0$, it holds for $k = k_0+1$ as well. In particular, (***) holds for $k = N-1$; performing the last integration in the same way as above we get (9) because $\Delta_N = \det M$. Finally if some of the principal minors are zero, then we replace M by $M_\varepsilon = M + \varepsilon I$. The above considerations are applicable to all but finite number of ε's , further $\lim_{\varepsilon\to 0} I_N(M_\varepsilon,\eta) = I_N(M,\eta)$ by the dominated convergence theorem, and therefore the assertion of Proposition 4 holds in this case too.

5. The propagator

The continuous contractive semigroup corresponding to our pseudo-Hamiltonian H can be expressed explicitly. This is the content of the following theorem, which shall be proved in the next section :

Theorem 2 : Let A, W be strictly positive and denote $\Omega = -(2B)^{1/2}$, $B = A - iW$. Then for each $t \geq 0$, $\exp(-iHt) = V_t$, where $\{V_t : t \geq 0\}$ is a contractive semigroup which acts on an arbitrary $\varphi \in L^2(\mathbb{R}^d)$ according to the relations

$$(V_t\varphi)(x) = \int_{\mathbb{R}^d} G_t(x,y)\,\varphi(y)\,dy \quad , \quad t > 0 \quad , \tag{12a}$$

$$G_t(x,y) = (2\pi i)^{-d/2}(\det(\Omega^{-1}\sin\Omega t))^{-1/2}\exp\Big\{\frac{i}{2}\Big[x.(\Omega\,\mathrm{ctg}\,\Omega t)x + y.(\Omega\,\mathrm{ctg}\,\Omega t)y\Big] - iy.(\Omega\,\mathrm{cosec}\,\Omega t)x\Big\} . \tag{12b}$$

One has to verify first that (12) makes sense :

Lemma 5.1 : Let A be positive, W strictly positive, $t > 0$, then Ω is regular and the real quadratic forms $x \mapsto -\mathrm{Im}\, x.(\Omega^{-1}\mathrm{tg}\,\Omega t)x$, $x \mapsto -\mathrm{Im}\, x.(\Omega\,\mathrm{tg}\,\Omega t)x$ and $x \mapsto \mathrm{Im}\, x.(\Omega\,\mathrm{ctg}\,\Omega t)x$ are strictly positive (positively definite in the algebraic terminology - cf. [20]).

Proof : Suppose first $d = 1$. We have $3\pi/2 \leq \arg B < 2\pi$ due to the assumption so that $0 < -\Omega_2 \leq \Omega_1$ holds for $\Omega = \Omega_1 + i\Omega_2$. Then

$$-\mathrm{Im}\,\Omega^{-1}\mathrm{tg}\,\Omega t = C(\Omega_2\,\mathrm{tg}\,\Omega_1 t\ \mathrm{ch}^{-2}\Omega_2 t - \Omega_1\,\mathrm{th}\,\Omega_2 t\ \cos^{-2}\Omega_1 t) \ ,$$

where $C^{-1} = |\Omega|^2\,|1 - i\,\mathrm{tg}\,\Omega_1 t\ \mathrm{th}\,\Omega_2 t|^2 > 0$. We abbreviate $\alpha_1 = 2\Omega_1 t$, $\alpha_2 = -2\Omega_2 t$: they are both positive, and therefore the inequalities $\alpha_1^{-1}\sin\alpha_1 < 1 < \alpha_2^{-1}\operatorname{sh}\alpha_2$ imply

$$-\operatorname{Im}\Omega^{-1}\operatorname{tg}\Omega t = C\left(4t\cos^2\left(\tfrac{1}{2}\alpha_1\right)\operatorname{ch}^2\left(\tfrac{1}{2}\alpha_2\right)\right)^{-1}(\alpha_1\operatorname{sh}\alpha_2 - \alpha_2\sin\alpha_1) > 0\ , \tag{13a}$$

$$\operatorname{Im}\Omega\operatorname{ctg}\Omega t = -|\Omega^{-1}\operatorname{tg}\Omega t|^{-2}\operatorname{Im}\Omega^{-1}\operatorname{tg}\Omega t > 0\ . \tag{13b}$$

Similarly, we obtain

$$-\operatorname{Im}\Omega\operatorname{tg}\Omega t > 0\ . \tag{13c}$$

Let further $d > 1$. Regularity of Ω is obvious : $|\Omega x|^2 = x.\Omega^T\Omega x = 2\,x.Bx \neq 0$ for non-zero $x \in \mathbb{R}^d$, because Ω is symmetric (as a function of symmetric B) and W is strictly positive. A real quadratic form is strictly positive, if all eigenvalues of its matrix are positive ([20], § X.5). They are equal to $-\operatorname{Im}\omega_j^{-1}\operatorname{tg}\omega_j t$ in the first case ([20], § V.1), where ω_j are eigenvalues of Ω. Further each eigenvalue $\beta_j = \frac{1}{2}\omega_j^2$ of B fulfils $\operatorname{Im}\beta_j < 0$, otherwise a nonzero x_{j_0} would exist such that $x_{j_0}.Wx_{j_0} = -\operatorname{Im}\beta_{j_0}|x_{j_0}|^2 \leq 0$ in contradiction with the assumption. Thus (13a) gives $-\operatorname{Im}\omega_j^{-1}\operatorname{tg}\omega_j t > 0$ for all j, and analogously (13b, c) apply to the other two forms. ■

<u>Lemma 5.2</u> : Let A, W be as in Lemma 5.1, then $\det(\Omega^{-1}\sin\Omega t)$ and $\det(\cos\Omega t)$ are non-zero for each $t > 0$.

<u>Proof</u> : It is sufficient to check that all eigenvalues of both the matrices are non-zero : they equal $\omega_j^{-1}\sin\omega_j t$ and $\cos\omega_j t$, $j = 1,\dots,d$, respectively. Further $\operatorname{Im}\beta_j < 0$ implies $\operatorname{Im}\omega_j \neq 0$, but sin and cos have no zeros outside the real axis. ■

<u>Proposition 5</u> : Let A, W be as in Lemma 5.1, let further V_t be given by (12) and $V_0 = I$. Then $\{V_t : t \geq 0\}$ is a semi-group of bounded operators on $L^2(\mathbb{R}^d)$.

<u>Proof</u> : According to Lemma 5.1 there exist positive c_1, c_2 (depending on t) such that

$$|G_t(x,y)| \leq c_1 \exp(-c_2(x^2+y^2))\ . \tag{14}$$

This inequality together with Fubini theorem implies

$$\|V_t\varphi\|^2 \leq c_1^2 \int_{\mathbb{R}^{3d}} |\varphi(y)|\,|\varphi(z)| \exp(-c_2(2x^2+y^2+z^2))\,dx\,dy\,dz =$$

$$= c_1^2\,(\pi/2c_2)^{d/2}\left(\int_{\mathbb{R}^d} |\varphi(y)| \exp(-c_2y^2)\,dy\right)^2$$

so that the Schwarz inequality gives

$$\|V_t\varphi\| \leq c_1(\pi/2c_2)^{d/2}\|\varphi\| \tag{15}$$

for each $\varphi \in L^2(\mathbb{R}^d)$. As for the semigroup property, in view of $V_0 = I$ and of (14) it is sufficient to verify

$$G_{t_1+t_2}(x,z) = \int_{\mathbb{R}^d} G_{t_2}(x,y)G_{t_1}(y,z)\,dy \tag{16}$$

for all $t_1, t_2 > 0$. The rhs of this relation equals

$$(2\pi i)^{-d}(\det(\Omega^{-1}\sin\Omega t_1)\det(\Omega^{-1}\sin\Omega t_2))^{-1/2}\exp\left\{\tfrac{i}{2}\left[x.(\Omega\,\mathrm{ctg}\,\Omega t_2)x + \right.\right.$$

$$\left.\left. + z.(\Omega\,\mathrm{ctg}\,\Omega t_1)z\right]\right\}.\ I_d(\Omega(\mathrm{ctg}\,\Omega t_1 + \mathrm{ctg}\,\Omega t_2), -\Omega((\mathrm{cosec}\,\Omega t_2)x + (\mathrm{cosec}\,\Omega t_1)z)).$$

Applying Proposition 4 to the last integral and using $\det M_1M_2 = \det M_1 \det M_2$, symmetry of the matrices involved and the matrix functional calculus rules([20] , § V.5), we get (16). ■

Before proceeding further, we shall deduce a useful equivalent expression for V_t :

<u>Proposition 6</u> : Let A, W be as in Lemma 5.1, then for all $t > 0$ and $\varphi \in L^2(\mathbb{R}^d)$

$$(V_t\varphi)(x) = \int_{\mathbb{R}^d} F_t(x,y)(F_d\varphi)(y)\,dy \quad , \tag{17a}$$

$$F_t(x,y) = (2\pi)^{-d/2}(\det(\cos\Omega t))^{-1/2}\exp\left\{-\tfrac{i}{2}\left[x.(\Omega\,\mathrm{tg}\,\Omega t)x + \right.\right.$$

$$\left.\left. + y.(\Omega^{-1}\mathrm{tg}\,\Omega t)y\right] + iy.(\sec\Omega t)x\right\} \quad , \tag{17b}$$

where F_d is the Fourier-Plancherel operator.

<u>Proof</u> : Let first $\varphi \in \mathcal{F}(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$, $\varphi(x) = \int_{\mathbb{R}^d} e^{ix.y}\,d\nu(y)$ with $\nu \in \mathcal{M}(\mathbb{R}^d)$, then (17a) can be rewritten as

$$(V_t\varphi)(x) = (2\pi)^{d/2} \int_{\mathbb{R}^d} F_t(x,y)\, d\nu(y) \quad . \tag{18}$$

In order to prove this, we use (14) together with boundedness of φ , $|\varphi(x)| \le |\nu|(\mathbb{R}^d)$. Then Fubini theorem applied to (12) gives (18) with

$$F_t(x,y) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} G_t(x,z)\, e^{iy.z}\, dz =$$

$$= (4\pi^2 i)^{-d/2} (\det(\Omega^{-1}\sin\Omega t))^{-1/2} \exp\left\{\frac{i}{2}\, x.(\Omega\,\mathrm{ctg}\,\Omega t)x\right\} .$$

$$. \, I_d(\Omega\,\mathrm{ctg}\,\Omega t\, , -(\Omega\,\mathrm{cosec}\,\Omega t)x) \quad .$$

Using now Proposition 4, symmetry of the matrices involved and the matrix functional-calculus rules, we get (17b).

Let us assume further an arbitrary $\varphi \in L^2(\mathbb{R}^d)$, and construct the following sequence :

$$\varphi_n : \varphi_n(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{ix.y}\, \hat{\varphi}_n(y)\, dy \quad ,$$

$$\hat{\varphi}_n(y) = \begin{cases} (F_d\varphi)(y) \;\ldots\; |y| \le n \text{ and } |(F_d\varphi)(y)| \le n \;, \\ n \;\ldots\ldots\; |y| \le n \text{ and } |(F_d\varphi)(y)| > n \;, \\ 0 \;\ldots\ldots\; |y| > n \;. \end{cases}$$

Clearly $F_d\varphi_n = \hat{\varphi}_n$ and $\hat{\varphi}_n \in L(\mathbb{R}^d)$ so the assertion is valid for φ_n . The sequence $\{\hat{\varphi}_n\}$ converges pointwise to $F_d\varphi$, further $|\hat{\varphi}_n(y)| \le |(F_d\varphi)(y)|$ and $F_t(x,.) \in L^2(\mathbb{R}^d)$ so that

$$\lim_{n\to\infty} (V_t\varphi_n)(x) = \int_{\mathbb{R}^d} F_t(x,y)(F_d\varphi)(y)\, dy \quad . \tag{*}$$

One verifies easily that $\hat{\varphi}_n \to F_d\varphi$ in the L^2-norm too. Since F_d is unitary and V_t is bounded due to (15), we obtain $V_t\varphi_n \to V_t\varphi$; then there exists a subsequence $\{V_t\varphi_{n_k}\}$ which converges to $V_t\varphi$ pointwise and the assertion follows from (*). ■

In order to prove Theorem 2 in a straightforward way, one has to check first that the semigroup $\{V_t : t \ge 0\}$ is strongly continuous, or equivalently

$$\lim_{t\to 0+} (\psi, V_t\varphi) = (\psi,\varphi) \tag{19}$$

for all $\psi,\varphi\in L^2(\mathbb{R}^d)$ ([22], Th.IX.1.1). Further the generator of $\{V_t : t\geq 0\}$ must be calculated and shown to coincide with H. According to Proposition 6, (19) is valid for $\psi,\varphi\in L^2(\mathbb{R}^d)\cap L(\mathbb{R}^d)$. Using further the matrix functional-calculus rules together with the relation

$$\frac{d}{dt}\det(g(\Omega t)) = \det(g(\Omega t))\, \mathrm{Tr}(\Omega g'(\Omega t)(g(\Omega t))^{-1}) \quad ,$$

one can verify that for $\varphi\in\mathcal{F}(\mathbb{R}^d)$, $\psi : \psi(x,t) = (V_t\varphi)(x)$ solves in $\mathbb{R}^d\times(0,\infty)$ the Schrödinger equation with the potential $v(x) = \frac{1}{2}\,x.\Omega^2 x$ and initial data φ.

The remaining part of such a proof, however, seems to be much more complicated. Instead of attempting it, we shall use the way which is opposite in some sense : to express $\exp(-iHt)$ by Lie-Trotter formula. This is the content of the next section.

6. exp(-iHt) by Lie-Trotter formula

We shall assume again both A,W to be strictly positive, $t>0$, and abbreviate $S_n^t = \exp(-iH_0t)\exp(-iVt)$, where $H_0 = \frac{1}{2}P^2$ is the free Hamiltonian. Since $iH = iH_0 + iV$ generates a continuous contractive semigroup due to Theorem 1, Lie-Trotter formula for semigroup asserts

$$\operatorname*{s-lim}_{n\to\infty} S_n^t = \exp(-iHt) \tag{20}$$

(cf. [23] or [14], Th.X.51 ; in fact we need only the special case of LT-formula considered by Nelson[13]). Our goal is to prove that the lhs of (20) coincides with V_t.

Let $\varphi\in L^2(\mathbb{R}^d)$, then using the propagator corresponding to H_0, one can express

$$(S_n^t\varphi)(x) = (2\pi i\delta)^{-nd/2}\int_{\mathbb{R}^{nd}}\exp\Big\{\frac{i}{2\delta}\sum_{k=0}^{n-1}(\gamma_{k+1}-\gamma_k)^2 - -i\delta\sum_{k=0}^{n-1}\gamma_k.B\gamma_k\Big\}\varphi(\gamma_0)\,d\gamma_0\ldots d\gamma_{n-1} \tag{21}$$

([14], Secs.IX.7, X.11), where $\gamma_n = x$ and $\delta = t/n$. Modulus of the integrand is majorized by

$$|\varphi(\gamma_0)| \ \exp\left\{-\delta \sum_{k=0}^{n-1} \gamma_k \cdot W\gamma_k\right\} \quad ,$$

thus the integral exists whenever $\varphi(.)$ is bounded and the integrations may be interchanged arbitrarily. In order to make use of Proposition 4 , suppose $\varphi \in \mathcal{F}(\mathbb{R}^d)$, $\varphi(x) = \int_{\mathbb{R}^d} e^{ix.x} d\nu(y)$. Substituting then $\gamma_k = \alpha_k \delta^{1/2}$, $k = 0,1,\ldots\ldots,n-1$, and rearranging the integral, we obtain

$$(S_n^t\varphi)(x) = (2\pi i)^{-nd/2} \int_{\mathbb{R}^d} d\nu(y) \exp(\tfrac{i}{2}\delta x^2)\, I_{nd}(M_n,\eta) \quad , \tag{22a}$$

where $\eta = (y\delta^{1/2},0,\ldots,0,-x\delta^{1/2})$ and $M_n = M_n(\delta)$ is the $nd \times nd$ matrix

$$M_n = \begin{pmatrix} I-2\delta^2 B & -I & 0 & 0 \ldots\ldots 0 \\ -I & 2I-2\delta^2 B & -I & 0 \ldots\ldots 0 \\ 0 & -I & 2I-2\delta^2 B & -I \ldots\ldots 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 \ldots\ 2I-2\delta^2 B \end{pmatrix} \tag{22b}$$

which obviously fulfils the asumptions of Proposition 4 . Further one has to calculate $\det M_n$ and M_n^{-1} (or at least its corner blocks). It can be accomplished, since the blocks in M_n commute mutually and thus can be handled ad numbers :

<u>Lemma 6.1</u> : Let $m = (m_{ij})$ be a $n \times n$ matrix and $M = (M_{ij})$ be a $nd \times nd$ matrix which consists of $d \times d$ blocks M_{ij} , $i,j = 1,2,\ldots,n$. Let us denote $d(m) = \mathcal{D}(m_{11},m_{12},\ldots,m_{nn}) := \det m$. If $[M_{ij},M_{kl}] = 0$, $i,j,k,l = 1,\ldots,n$, then

$$\det M = \det(d(M)) \quad , \tag{23a}$$

where $d(M)$ is the "block determinant" of M , i.e., the $d \times d$ matrix $\mathcal{D}(M_{11},M_{12},\ldots,M_{nn})$. Moreover, if M is regular, then

$$(M^{-1})_{ij} = (-1)^{i+j}(d(M))^{-1} M\begin{bmatrix} 1,\ldots,j-1,j+1,\ldots,n \\ 1,\ldots,i-1,i+1,\ldots,n \end{bmatrix} \quad , \tag{23b}$$

where $M[\ldots]$ is the respective "block minor" of M , i.e., $d(\widetilde{M}_{ij})$ with $\widetilde{M}_{ij}$ obtained from M by dropping the j-th "block row" and the i-th "block column".

<u>Proof</u> : For $n = 2$ see [20] , § II.5, in particular (23b) follows

from Frobenius formula. The determinant (23a) can be evaluated using the block variant of Gauss algoritm :

$$\det M = \det \tilde{M} \quad , \quad \tilde{M} = M_{11}M_{22}^{(1)}M_{33}^{(2)}\dots M_{nn}^{(n-1)} \quad ,$$

where $M_{ij}^{(k)} = M_{ij}^{(k-1)} - M_{ik}^{(k-1)}(M_{kk}^{(k-1)})^{-1}M_{kj}^{(k-1)}$, $i,j = k+1,\dots,n$, $k = 1,2,\dots,n-1$. Since all the blocks commute, we see that $\tilde{M}$ is the same polynomial function of variables M_{ij} as $d(m)$ of m_{ij}, i.e., that $\tilde{M} = d(M)$. Notice that this is true even if some $M_{kk}^{(k-1)}$ is singular (by the ε-trick : cf. proof of Proposition 4). Further (23b) is equivalent to the relation

$$\sum_{j=1}^{n} (-1)^{i+j} \, M\begin{bmatrix} 1,\dots,j-1,j+1,\dots,n \\ 1,\dots,i-1,i+1,\dots,n \end{bmatrix} M_{jk} = \delta_{ik}\, d(M)$$

which follows similarly from the analogous equality for the matrix m . ∎

Using this lemma, the needed blocks of M_n^{-1} are easily calculated, giving thus

$$(S_n^t\varphi)(x) = (\det[d(M_n)])^{-1/2} \int_{\mathbb{R}^d} d\nu(y) \, \exp\Big\{ -\frac{i}{2\delta}\, x.d(M_n)^{-1}\big[d(M_{n-1}) - - d(M_n)\big]x - \frac{i\delta}{2}\, y.d(M_n)^{-1} d(K_{n-1})y + i\,y.d(M_n)^{-1}x \Big\} \,, \tag{24}$$

where $K_{n-1} = K_{n-1}(\delta)$ is the abbreviation for the lower-right $(n-1)d \times (n-1)d$ submatrix of M_n . The "block determinants" under consideration obey the following relations

$$d(M_n) = (I - \delta^2\Omega^2)d(K_{n-1}) - d(K_{n-2}) \quad , \tag{25a}$$

$$d(K_{n-1}) = (2I - \delta^2\Omega^2)d(K_{n-2}) - d(K_{n-3}) \quad . \tag{25b}$$

One can verify directly that the recursive relation (25b) is solved by

$$d(K_{n-1}) = \sum_{j=0}^{\infty} (-1)^j \binom{n+j}{2j+1} (\delta\Omega)^{2j} \quad ; \tag{26}$$

substituting it into (25a), we get

$$d(M_n) = \sum_{j=0}^{\infty} (-1)^j \binom{n+j}{2j} (\delta\Omega)^{2j} \quad . \tag{27}$$

Let us turn now to the limits. Assume first $\delta d(K_{n-1}(\delta))$ with $\delta = t/n$: this sum converges (because it is finite), however, one must verify that it converges uniformly with respect to n . It holds

$$\frac{t}{n}\, d(K_{n-1}(\tfrac{t}{n})) = \Omega^{-1} \sum_{j=0}^{\infty} \frac{(-1)^j}{(2j+1)!}\, c_{nj} (\Omega t)^{2j+1} \quad ,$$

where $c_{nj} = \prod_{k=1}^{j} (1-k^2 n^{-2})$ so that $0 \le c_{nj} \le 1$ for all n,j , and therefore the convergence is uniform. Thus we have

$$\lim_{n\to\infty} \frac{t}{n}\, d(K_{n-1}(\tfrac{t}{n})) = \Omega^{-1} \sin \Omega t \quad ; \tag{28}$$

similarly one obtains

$$\lim_{n\to\infty} d(M_n(\tfrac{t}{n})) = \cos \Omega t \quad , \tag{29}$$

$$\lim_{n\to\infty} \frac{n}{t} \left[d(M_{n-1}(\tfrac{t}{n})) - d(M_n(\tfrac{t}{n}))\right] = \Omega \sin \Omega t \quad . \tag{30}$$

These relations together with (24),(17b),(18) and the matrix functional-calculus rules give

$$\lim_{n\to\infty} (S_n^t \varphi)(x) = (V_t \varphi)(x) \tag{31}$$

for $\varphi \in \mathcal{F}(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$. On the other hand, $\lim_{n\to\infty} S_n^t \varphi = \exp(-iHt)\varphi$ for these φ due to (20) so that there exists a subsequence $\{S_{n_k}^t \varphi\}$ which converges to $\exp(-iHt)$ pointwise a.e. in $\mathbb{R}^d$. Consequently, we have

$$V_t \varphi = \exp(-iHt)\varphi \tag{32}$$

for all $\varphi \in \mathcal{F}(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$. This set is, however, dense in $L^2(\mathbb{R}^d)$ (containing, e.g., $\mathcal{S}(\mathbb{R}^d)$) and the operators V_t , $\exp(-iHt)$ are bounded due to Proposition 5 and Theorem 1 , respectively, thus (32) holds for each $\varphi \in L^2(\mathbb{R}^d)$ too and the proof of Theorem 2 is finished.

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