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LIFETIME OF LOCALIZED STATES FOR A GENERALIZED SCHRÖDINGER OPERATOR APPEARING IN NUCLEAR PHYSICS

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Abstract. We apply time-energy uncertainty inequalities introduced by Pfeifer and Fröhlich [27] to estimate the lifetime of quasistationary mixed states for a variable coefficients Schrödinger operator, without using directly resonance theory.

1. Introduction

In various phenomena of quantum physics one is interested in the dynamics of quantum states driven by Schrödinger operators with variable coefficients and made unstable due to tunneling.

The first example comes from quantum field theory on curved spaces (Riemanian manifolds) where barrier penetration may justify the decay of "false vacua" [8, 6, 13]. Just mention that in cosmology, tunelling of such false vacua could explain nucleation processes during the formation of the early universe [31, 35].

A second example comes from low-energy nuclear physics [7, 19, 20, 28] where the study of large collective motions of a heavy nucleus made of N nucleons (protons and neutrons) is investigated by the so called Generator Coordinate Method (GCM) [29]. Namely taking weighted superpositions of collective coordinates as trial functions for deformed states and applying a minimization precedure, one gets the Hill and Wheeler non-local integral equation [18], which in turn, after solving in the so-called Gaussian Overlap Approximation (GOA) [36], reduces to a 1 body problem described by a Schrödinger equation in $\mathbb{R}^d$ with variable coefficients (d is the number of collective degrees of freedom which, in the present status of computations [14], is currently in the range 1-5).

The simplest paradigm for quantifying these decay phenomena is the so called "puits dans l'isle" problem introduced by Helffer and Sjöstrand in [16] which reads as follows: " given a potential with a local minimum and decaying at large distance, try to estimate the "life time" T of an unstable state escaping from the well surrounding the local minimum".

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In a physical (formal) setting, functional integral formalism [37] gives a formula for such a lifetime T, of the type

$$T = A\, e^{\frac{B}{\hbar}}, \tag{1.1}$$

where A, B are positive constants partially computable in some specific situations (see [8, 6]) and the exponential is expected to be large due to the presence of the small parameter $\hbar$ (Planck's constant).

From a mathematical point of view the main strategy invoked to make (1.1) rigorous is to identify the lifetime T as the inverse of the imaginary part of a resonance Γ as in [10, 22, 25, 34] in a time-dependent process and to estimate the width Γ by using the now well-developed semiclassical resonance theory based on complex deformations (see [9, 11, 16, 17] for detailed expositions).

In fact an equality such that (1.1) is out of reach, at least in the multidimensional case ($d > 1$) and only upper (and sometimes lower) bounds for Γ have been proved by Helffer and Sjöstrand [16] (see also [24]) for arbitrary $d \geq 1$.

Alternatively, another possible definition of lifetime can be derived from first principles through a direct estimate of the probability $p(t) = \mathrm{Trace}(P\rho(t))$ for a quantum system described by the density operator $\rho(t)$ at time t to remain in a given subspace of the state space $\mathcal{H}$ defined by the projector P on suitable subspaces.

This last approach has been introduced by Pfeifer and Fröhlich [27] and applied in [1] to adiabatic evolutions, with the advantage that it does not rely directly on resonance theory and avoid technical assumptions on operators in the (non physical) complex domain.

In [5] we considered an extension of the first method to a Schrödinger operator with variable coefficients and then evaluated the lifetime as the inverse of the imaginary part of the associated resonance.

In the present note, we focus on the second method and we show that the robust estimates of Pfeifer and Fröhlich in [27], relying on suitable time-uncertainty relations, can also be adapted to the generalized (variable coefficients) Schrödinger case to recover an upper bound of the type (1.1) for some (in principle calculable) positive numbers A and B depending on the geometry of the problem.

The plan of the paper is as follows: in Section 2 we define the model, in Section 3 we introduce a comparison dynamics and derive necessary estimates for the various operators involved, then in Section 4 we give and prove our main result by applying a time-energy uncertainty relation proposed in [27] and recalled for the reader's convenience in the Appendix. In the whole paper we shall use the Einstein's summation convention on repeated indices.

2. Physical model

As presented in the introduction, our model is issued from low-energy nuclear physics and the Generator Coordinate Method leads to a Schrödinger operator with variable coefficients in $\mathbb{R}^d$, where d is the number of degrees of freedom so we define the hamiltonian of the system by

$$H(\lambda) := -g^{-1/2}(x)\partial_j(g^{1/2}(x)g^{jk}(x)\partial_k) + V_\lambda(x), \tag{2.1}$$

where $V_\lambda(x) := \lambda^2 V(x)$.

In (2.1) λ is a large positive parameter (in the semiclassical context, one can think to $\lambda = \frac{1}{\hbar}$), $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ represents collective variables (physically:

multipolar momenta) with $\partial_k = \frac{\partial}{\partial x_k}$, $k = 1, \dots, d$ and $g_{ij}(x)$ is the collective "mass tensor" with $g_{ij}g^{jk} = \delta_i^k$ (Kronecker's index), $i, k = 1, \dots, d$ and $g(x) = \det\{g^{jk}(x)\}$.

In fact from a computational point of view the functions $V(x_a)$ and $g_{ij}(x_a)$ are obtained from a finite number of (constrained) mean field calculations based on Hartree-Fock-Bogoliubov approximation [29], for each x_a in a finite set $F \subset \mathbb{R}^d$ (see [7] for a brief description of such a computation). However we will assume in the following that $V(x)$ and $g_{ij}(x)$ are smooth functions defined for any $x \in \mathbb{R}^d$, even for large x where the approximation is questionable.

Supposing that the function V has a local minimum corresponding to a metastable collective state of the nucleus and that the barrier separating this local minimum from the exterior world is large and high enough (observe that the height of the barrier is $\mathcal{O}(\lambda^2)$ and that its diameter and width are $\mathcal{O}(\lambda)$) one expects that any quantum collective states initially trapped in the local well will spend a long time in it and will ultimately escape outside by tunnelling through the barrier.

In the nuclear context the local minimum may correspond to an unstable nucleus decaying into several fragments through a fission barrier [20, 28] or it can also correspond to a state of spherical shape of the nucleus (unstable for a large class of heavy nuclei) tunelling through the barrier toward a (super-)deformed state [7].

After definition (2.1), it is natural to think of the previous quantum dynamics as taking place on a Riemannian manifold (X, g) [33] provided with the Riemannian metric g given in local coordinates by $g^{ij} \in C^\infty(X)$ and associated distance d_g. Setting $g(x) = \det(g^{ij}(x))$ and $g_{ij}g^{jk} = \delta_i^k$ with (Kronecker's index), $i, k = 1, \dots, d$, where the summation convention is used, the (generalized) Schrödinger operator H in (2.1) is

$$H(\lambda) = -\frac{1}{2}\Delta_g + V_\lambda, \tag{2.2}$$

where Δ_g is the Laplace-Beltrami operator locally defined for any $u \in C^\infty(X)$ by

$$\Delta_g u := g^{-1/2}\partial_j(g^{1/2}g^{jk}\ \partial_k u). \tag{2.3}$$

This geometric framework has been used in the "resonance" point of view by De Bièvre-Hislop [3] and Froese-Hislop [12], however in the present note we do not focus on the global geometrical aspects of the problem and concentrate on the variable coefficient framework so we will suppose in all the sequel that $X \equiv \mathbb{R}^d$ and $H(\lambda)$ is the variable coefficient elliptic operator defined globally on $X \equiv \mathbb{R}^d$ by (2.2) and (2.3). Accordingly we denote by $L^2(X)$ the weighted space $L^2(\mathbb{R}^d, dV_g)$ with $dV_g(x) = g(x)\,dx$ and by H^s for $s \in \mathbb{R}$ the associated Sobolev spaces built on $L^2(\mathbb{R}^d, dV_g)$.

3. Comparison dynamics

3.1. **Comparison dynamics and spectral properties.** According to the previous presentation we suppose that $g^{ij}(x) \sim \delta^{ij}$ (Kronecker symbol) for $|x|$ large ("$X \equiv (\mathbb{R}^d, g)$ is euclidean at large distance") and we note $|x| = d_g(0, x)$ for any $x \in X$. For a multiindex $\alpha \in \mathbb{N}^d$ with $|\alpha| := \sum_{j=1}^d \alpha_j$, we note $D_x^\alpha = \partial_{x_1}^{\alpha_1}\partial_{x_2}^{\alpha_2}\dots\partial_{x_d}^{\alpha_d}$.

More precisely we suppose that there exist positive constants R, C_α, $C_{R,\alpha}$ and ε such that

(A1) The matrix $\{g^{ij}\}$ is positive definite and smooth: $g^{ij} \in C^\infty(X)$. Moreover

$$|D_x^\alpha g^{ij}(x)| \leq C_\alpha, \tag{3.1}$$

for $|\alpha| = 0, 1, 2$ and $i, j = 1, \dots, d$,

(A2) The matrix $\{g^{ij}\}$ decays toward identity at large distance

$$|D_x^\alpha (g^{ij}(x) - \delta^{ij})| \le C_{\alpha,R} \langle x \rangle^{-|\alpha|-\varepsilon}, \tag{3.2}$$

for any $|x| \ge R$, for $|\alpha| = 0, 1, 2$ and $i, j = 1, \dots, d$, with $\langle x \rangle := (1+|x|^2)^{-1/2}$ and a possibly small $\varepsilon > 0$ (long range case).

We also suppose that the potential V is smooth, of shape-resonance type ("le puits dans l'isle" in the terminology of Helffer and Sjöstrand [16]) and is small at large distance.

Namely there exist positive constants R and $C'_{R,\alpha}$ such that

(A3) $V \in C^\infty(X)$, $V \ge 0$.

(A4) V has a positive non degenerate local minimum V_0 at the origin: $V_0 = V(0) > 0$.

(A5) V goes to zero at large distance:

$$|D_x^\alpha V| \le C'_{R,\alpha} \langle x \rangle^{-|\alpha|-\varepsilon} \quad \text{for } |x| > R \text{ and } |\alpha| = 0, 1, 2,$$

for a possibly small $\varepsilon > 0$ (long range potential).

(A6) For a small $w > 0$ precised below, the classically forbidden region (see [17] Chap. 20)

$$\mathcal{F}(V_0 + w) := \{x \in \mathbb{R}^d : \ V(x) > V_0 + w\},$$

is a relatively compact region bounded by two smooth hypersurfaces $S^-(V_0+w)$ and $S^+(V_0+w)$ (turning surfaces) such that the interior region $\mathcal{W}(V_0+w)$ (the well) is bounded by $S^-(V_0 + w)$ and the exterior (unbounded) region $\mathcal{E}(V_0 + w)$ admits $S^+(V_0 + w)$ as boundary.

Provided λ is large enough, one expects that the well $\{|x| \ll R\}$ and the exterior region $\{|x| \gg R\}$ are almost decoupled, and we define a comparison potential

$$\widetilde{V}(x) = \begin{cases} V_0 + w & \text{for } x \in \mathcal{E}(V_0 + w), \\ V(x) & \text{for } X \backslash \mathcal{E}(V_0 + w), \end{cases}$$

where we suppose that w is small enough in order that $\tilde{V}$ has a ground state E_0 such that $V_0 < E_0 < V_0 + w$.

The corresponding comparison hamiltonian is then defined as

$$H_0(\lambda) := -g^{-1/2}(x)\partial_j(g^{1/2}(x)g^{jk}(x)\partial_k) + \widetilde{V}_\lambda(x) \equiv -\frac{1}{2}\ \Delta_g + \lambda^2 \widetilde{V}(x), \tag{3.3}$$

and we denote by W_λ the perturbation

$$W_\lambda(x) = V_\lambda(x) - \widetilde{V}_\lambda(x). \tag{3.4}$$

It is well known [33] that $H(\lambda)$ and $H_0(\lambda)$ are well defined as selfadjoint operators on $L^2(X)$ with domain $H^2(X)$ and we first briefly describe their spectra.

Lemma 3.1. *Under assumption* (A3) *on the potential V, $H(\lambda)$ and $H_0(\lambda)$ are bounded below. Moreover*

1. *For each $\alpha < w$: $\sigma_d(H_0) \equiv \sigma(H_0) \cap (-\infty, \alpha))$ consists of a finite number of eigenvalues e_n of finite multiplicity.*
2. $\sigma_{\rm ess}(H_0(\lambda)) = [\lambda^2(V_0 + w), \infty)$.
3. $\sigma(H(\lambda)) = \sigma_{\rm ess}(H(\lambda)) = [0, \infty)$.
4. *Singular continuous spectra $\sigma_c(H(\lambda))$ and $\sigma_c(H_0(\lambda))$ are empty.*

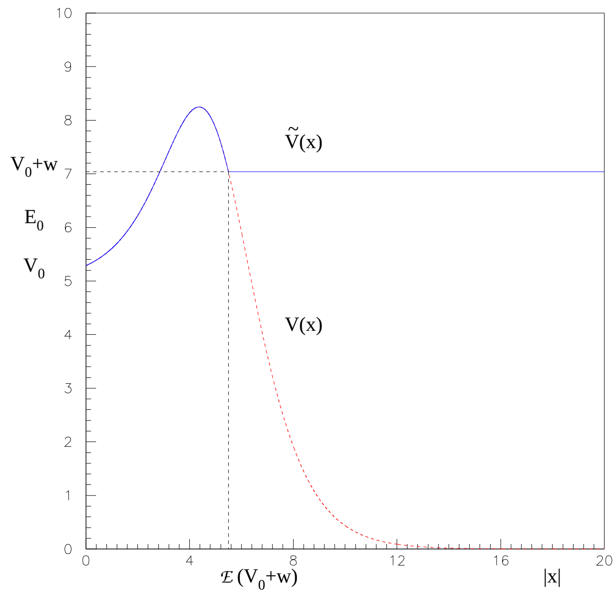

FIGURE 1. Comparison potential $\widetilde{V}(x)$.

Proof. 1. Given any energy E such that $V_0 < E < V_0 + w$, there is a finite set $\mathcal{E}_E$ of eigenvalues e_n of H_0 such that

$$e_n < E \quad \text{for } |n| \le N_E := \operatorname{card}(\mathcal{E}_E).$$

Moreover using a generalization of the Cwikel-Lieb-Rosenblum estimate [26], one has the "explicit" bound for N_E, namely

$$N_E \le \frac{1}{g(1)} \int_0^\infty \int_X p(t;x,x) G(\lambda^2 t(\widetilde{V} - E)_-) dV_g(x) \frac{dt}{t}, \tag{3.5}$$

where G is any arbitrary non trivial convex function on $[0,\infty)$ polynomially bounded and such that $s \to s^{-1}G(s)$ is integrable near 0, $g(1)$ is the Laplace transform of $s \to s^{-1}G(s)$ and $p(t;x,y)$ is the heat kernel for Δ_g defined by $e^{-t\Delta_g} f(x) = \int_X p(t;x,y) f(y) dV_g(y)$. As the integral is convergent, N_E is finite.

2. It will be convenient to shift the potential to fix it at 0 at infinity. So we put $\widehat{V}(x) := \widetilde{V}(x) - \lambda^2(V_0 + w)$ and the shifted comparison hamiltonian is then $\widehat{H}_0 = -\frac{1}{2}\Delta_g + \widehat{V}$.

After Step 1. we know that $\sigma_{\rm ess}(\widehat{H}_0(\lambda)) \cap (-\infty, 0) = \emptyset$, so we have just to prove that $[0,\infty) \subset \sigma(\widehat{H}_0)$. We know that $\lambda \ge 0$ belongs to $\sigma(\widehat{H}_0)$ if and only if (Weyl's criterion) there is a sequence $\phi_n \in D(\widehat{H}_0)$, $n \in \mathbb{N}^d$ such that

$$\lim_{n\to\infty} \frac{\|(\widehat{H}_0 - \lambda I)\phi_n\|}{\|\phi_n\|} = 0. \tag{3.6}$$

To construct such a sequence, one observes that

$$-\Delta_g e^{ik\cdot x} = (-ik_j\partial_i g^{ij} + k_ik_jg^{ij} - \frac{i}{2}\ k_j\partial_i(\log g)g^{ij})e^{ik\cdot x},$$

so as $\widehat{V}(x) \to 0$ at infinity,

$$\lim_{|x|\to\infty} \big[-\frac{1}{2}\Delta_g + \widehat{V} + ik_j\partial_i g^{ij} - k_ik_jg^{ij} + \frac{i}{2}\ k_j\partial_i(\log g)g^{ij}\big]e^{ik\cdot x} = 0.$$

Let us pick a cut off $\chi \in C_0^\infty(X)$ such that $\chi(x) \ge 0$, $\chi(x) = 1$ for $|x| \le 1/2$ and $\chi(x) = 0$ for $|x| \ge 2$ and set $\chi_n(x) := \chi(|n|^{-1/2}(x-n))$ for $n \in \mathbb{Z}^d$. Of course $\operatorname{supp}\chi_n \subset \{x \in X : \ |x-n| \le |n|^{1/2}\}$ therefore

$$\lim_{|n|\to\infty} \sup_{x\in\operatorname{supp}\chi_n} |\widehat{V}| = 0.$$

It is easy to check that the sequence $\{\phi_n\}_n$ such that $\phi_n(x) = \chi_n(x)e^{ik\cdot x}$, with k such that $\lambda = \sup_{x\in X} g^{ij}(x)k_ik_j$, satisfies (3.6).

3. As $V > 0$, $\sigma_{pp}(H(\lambda)$ is empty after the Cwikel-Lieb-Rosenblum bound on the number of eigenvalues, moreover for $\sigma_{\rm ess}(H(\lambda))$ the same proof as that given in Step 2. (with $w = 0$) applies.

4. Let $H = H(\lambda)$ or $\widehat{H}_0(\lambda)$. After [30, Theorem XIII.19] it is sufficient to show that for any interval $(\mu_1,\mu_2) \in \mathbb{R}_+$ the bound $\sup_{\varepsilon>0}\sup_{\mu\in(\mu_1,\mu_2)} |\langle f, \Im m(H-\mu-i\varepsilon)^{-1}f\rangle| \le C(f) < \infty$ holds for f in a dense set of $L^2(X)$ but after the decay property (A2) assumed above for g^{ij}, for positive energies, this estimate follows from [32, Proposition 1.1] and for small non negative energies, after [4, Theorem 12]. □

Remark 3.2. It can also be checked that embedded eigenvalues are absent from $\sigma_{\rm ess}(H(\lambda))$ and from $\sigma_{\rm ess}(H_0(\lambda))$. In fact after the decay properties (A2) and (V_3), one can directly use a result of Koch and Tataru [23] (indeed the original argument of [23] involving the hamiltonian $-\partial_j(g^{jk}\partial_k u) + V$ extends without modification to $-\Delta_g u + Vu$).

Namely, let us denote $L := \frac{1}{2}\Delta_g$ and $V := V_\lambda + E$ for a positive E. We assume that for a $\delta > 0$ small enough:

$$\limsup_{|x|\to\infty} |x||Dg^{ij}(x)| \le \delta, \quad \liminf_{|x|\to\infty} V > 0, \quad \tau_0 := -\liminf_{|x|\to\infty} \frac{x\cdot\nabla V}{4V} < 1/2.$$

So supposing that $u \in H^1_{\rm loc}$ is a solution of $Lu + Vu = 0$ with $|u|^{\tau_1-1/2} \in L^2$ for a $\tau_1 > \tau_0$, we conclude from [23, Theorem 12] that $u \equiv 0$, which of course excludes that E is an eigenvalue.

3.2. **Exponential decay of eigenfunctions of H_0.** In the sequel, we use the simplified notation: V for V_λ and $\widetilde{V}$ for $\widetilde{V}_\lambda$.

Following Agmon [2] we denote by $\rho_A(x,y;V,E)$ the Agmon's distance in X at energy $E > 0$ corresponding to the potential V, associated to the Riemannian metric $ds^2 = (V(x)-E)_+g_{ij}(x)\,dx_i\,dx_j$, where $\{g_{ij}\} := \{g^{ij}\}^{-1}$, given for any pair $x, y \in X$ by

$$\begin{aligned}&\rho_A(x,y;V,E)\\ &:= \inf_{\{\gamma\in AC[0,1]:\gamma(0)=x,\gamma(1)=y\}} \int_0^1 [V(\gamma(t))-E)_+]^{1/2}[g_{ij}(\gamma(t))\dot\gamma_i(t)\dot\gamma_j(t)]^{1/2}dt.\end{aligned} \tag{3.7}$$

Assuming that the classically forbidden region $\mathcal{F}_V(E) := \{x \in X : V(x) > E\}$ at energy E separates X into two disjoint connected sets: the (bounded) well $\mathcal{W}_V(E)$ with boundary $S_V^-(E)$ and the (unbounded) exterior region $\mathcal{E}_V(E)$ with boundary $S_V^+(E)$, the associated distance from $S_V^-(E)$ to $S_V^+(E)$ is defined by

$$\rho_A(V;E) = \inf_{x\in S_V^-(E), y\in S_V^+(E)} \rho_A(x,y;V,E). \tag{3.8}$$

Of course one defines as well the analogous quantities corresponding to the approximate potential $\widetilde{V}$, and in this case we will omit in the sequel the argument $\widetilde{V}$.

Then we write $\rho_A(x,y;E)$ for $\rho_A(x,y;\widetilde{V},E)$, $\mathcal{W}(E)$ for $\mathcal{W}_{\widetilde{V}}(E)$, $S^-(E)$ for $S^-_{\widetilde{V}}(E)$ and $\mathcal{F}(E)$ for $\mathcal{F}_{\widetilde{V}}(E)$. We also use the notation $\rho_A(x;V,E) := \rho_A(x,0;V,E)$.

Suppose now that n is such that the classically forbidden region $\mathcal{F}(e_n)$ at energy $e_n := e_n(\lambda) \in \sigma(H_0)$ is not empty and that $\partial B(0,R) \subset \mathcal{F}(e_n)$ for any λ large enough.

Theorem 3.3. *Suppose that ψ is an eigenfunction of H_0 associated to the eigenvalue $e_n$and let $\varepsilon > 0$ be arbitrary small. There exists a constant $C_n > 0$ independent of λ such that for any λ large enough,*

$$\|e^{(1-\varepsilon)\rho_A(\cdot;\widetilde{V},e_n)}\ \psi\|_{L^2(X)} \le C_n.$$

Proof. As the proof can be easily adapted from Hislop-Sigal [17], using complementary arguments of Agmon [2] in the variable coefficient case (see also Helffer [15]) we just sketch the main points.

(1) The mapping $x \to \rho_A(x,y;\widetilde{V},e_n)$ is locally Lipschitz continuous and then differentiable almost everywhere in each variable. Moreover at any point x where it is differentiable, the Eikonal inequality holds $|(\nabla_g)_x\rho_A(x,y;\widetilde{V},e_n)|^2 \le (\widetilde{V}(x) - e_n)_+$, for any $y \in X$ and $e_n \in \sigma(H_0)$. Moreover the function $E \to \rho_A(x,y;\widetilde{V},E)$ is increasing.

(2) For any fixed $\epsilon, \delta > 0$ small enough, let $E := e_n$ and $f(x) := (1-\epsilon)\rho_A(x;\widetilde{V},E)$ and let $\phi \in D(\widetilde{V}) \cap H^1(X)$ compactly supported in the set $\mathcal{F}_{E<\delta} \equiv \{x \in X : \widetilde{V}(x) - E > \delta\}$. Then, using Step 1, there exists a positive constant δ_1 such that

$$\mathrm{Re}\langle e^f\phi, (H_0 - E)e^{-f}\phi\rangle \ge \delta_1\|\phi\|^2. \tag{3.9}$$

(3) Let $\alpha > 0$, $E := e_n$ and $f_\alpha = f(1+\alpha f)^{-1}$ and let θ be a smooth bounded function such that $|\nabla_g\theta|$ is compactly supported. Defining $\phi \equiv \theta e^{f_\alpha}\psi$, where $H_0\psi = E\psi$, one checks that

$$\mathrm{Re}\langle e^{f_\alpha}\phi, (H_0 - E)e^{-f_\alpha}\phi\rangle = \langle \xi e^{2f_\alpha}\psi, \psi\rangle, \tag{3.10}$$

where $\xi = |\nabla_g\theta|^2 + 2\theta\nabla_g\theta\cdot\nabla_g f_\alpha$.

(4) Let us consider for $E := e_n$ the sets

$$\mathcal{F}_{E,2\delta} := \{x \in X : \widetilde{V}(x) - E > 2\delta\}, \quad \mathcal{A}_{E,\delta} := \{x \in X : \widetilde{V}(x) - E < \delta\},$$

associated to $E \in \sigma_d(H_0)$ and let $\theta \in C^\infty(X)$ be such that

$$\theta(x) = \begin{cases} 1 & \text{if } x \in \mathcal{F}_{E,2\delta}, \\ 0 & \text{if } x \in \mathcal{A}_{E,\delta}. \end{cases}$$

After the construction of $\widetilde{V}$, $\nabla_g\theta$ is compactly supported. Let $f = (1-\epsilon)\rho_A(E)$ and $f_\alpha = f(1+\alpha f)^{-1}$ as before. Then $\phi = \theta e^{f_\alpha}\psi$ meets the hypotheses of Step 2. so using (3.9) there exists a positive δ_1 such that

$$\delta_1\|\phi\|^2 \le \mathrm{Re}\langle e^{f_\alpha}\phi, (H_0-E)e^{-f_\alpha}\phi\rangle \le |\langle \xi e^{f_\alpha}\psi, \psi\rangle| \le \sup_{x\in\mathrm{supp}\,|\nabla_g\theta|} |\xi e^{2f_\alpha}|\|\psi\|^2, \tag{3.11}$$

where we used (3.10). As $\nabla_g\theta$ is compactly supported, we can take $\alpha = 0$ in the right hand side of (3.11). If $f_0 \equiv \sup_{x\in\mathrm{supp}\,|\nabla_g\theta|}|f(x)|$ and for a normalized ψ

$$\|e^{f_\alpha}\theta\psi\|^2 \le C, \tag{3.12}$$

for a $C > 0$ independent of α. So we can take $\alpha = 0$ in the left hand side of (3.12).

Now as $S_\delta := \mathrm{supp}\,|\nabla_g\theta| \cup \overline{\mathcal{A}}_{E,\delta}$ is compact, $e^{2f(x)}$ is bounded on this set and $\int_S e^{2f}|\psi|^2\,dV_g(x) < \infty$. Then finally there exists $C_{\varepsilon,n} \in (0,\infty)$ such that

$$\begin{aligned}
&\int e^{2(1-\epsilon)\rho_A(x,E)}|\psi(x)|^2\,dV_g(x)\\
&= \int_{\{x:\theta(x)=1\}} e^{2f}|\psi(x)|^2\,dV_g(x) + \int_{S_\delta} e^{2f}|\psi(x)|^2\,dV_g(x) \le C_{\varepsilon,n},
\end{aligned}$$

which completes the proof by taking the best constant $C_{\varepsilon,n}$. □

4. Lifetime of a quasi-localized state

In the sequel, we note H and H_0 for $H(\lambda)$ and $H_0(\lambda)$. After Lemma 3.1, given any energy E such that $V_0 < E < V_0 + w$, there is a finite set $\mathcal{E}_E$ of eigenvalues e_n of H_0 such that $e_n < E$ for $|n| \le N_E := \mathrm{card}(\mathcal{E}_E)$. Denoting by ψ_n the associated eigenfunctions and $\mathcal{H}_E$ the subspace of $\mathcal{H}$ spanned by the set $\{\psi_n; |n| < N_E\}$, let us define a closed complex contour $\gamma_E \in \mathbb{C}$ such that its interior Δ_E contains the discrete set $\sigma_0 \cap [0,E]$ where σ_0 is the spectrum of H_0, and such that the distance from γ_E to σ_0 satisfies

$$\mathrm{dist}(\gamma_E,\sigma_0) := \delta_E = \frac{1}{2}\min_{|n|,|n'|\le N_E}|e_n - e_{n'}| > 0. \tag{4.1}$$

The spectral projector of H_0 on the subspace $\mathcal{H}_E$ is the Riesz integral

$$P_{\lambda,E} = \frac{1}{2\pi i}\int_{\gamma_E}(z-H_0)^{-1}dz, \tag{4.2}$$

with $\mathrm{tr}(P_{\lambda,E}) = N_E$.

Lemma 4.1. *For any $\phi \in \mathrm{Ran}(P_{\lambda,E})$ there exists a real positive constant C_E such that*

$$\|e^{(1-\varepsilon)\rho_A(\cdot;\widetilde{V},e_N)}\phi\|_{L^2(X)} \le C_E\|\phi\|_{L^2(X)}. \tag{4.3}$$

Proof. Let $\Phi_E(x) := e^{(1-\varepsilon)\rho_A(\cdot;\widetilde{V},e_N)}$ and $\phi \in \mathcal{H}_E$ with $\phi := \sum_{n=1}^{N_E}\lambda_n\psi_n$. One has

$$\begin{aligned}
\int_X |\Phi_E\phi|^2 dV_g(x) &= \int_X |\Phi_E|^2|\sum_{n=1}^{N_E}\lambda_n\psi_n|^2 dV_g(x)\\
&\le \|\phi\|^2_{L^2(X)}\int_X|\Phi_E|^2\sum_{n=1}^{N_E}|\psi_n|^2\,dV_g(x),
\end{aligned}$$

and (4.3) follows from Theorem 3.3. □

Recall that the density operator ρ_t associated to H is solution of the Liouville equation $i\lambda\partial_t\rho_t = [H, \rho_t]$ with $\rho_t|_{t=0} = \rho_0$. Our main result is the following.

Theorem 4.2. *Suppose that $P_{\lambda,E}$ is the projector defined by* (4.2) *and suppose that we prepare the initial density operator ρ_0 of the system according*

$$\operatorname{tr}(\rho_0 P_{\lambda,E}) \geq (1-\boldsymbol{\epsilon})^2,$$

for a small $\boldsymbol{\epsilon} > 0$. Then the probability $p_t := \operatorname{tr}(\rho_t P_{\lambda,E})$ for the density operator ρ_t to remain in the range of the projector $P_{\lambda,E}$ is bounded as follows

$$\sin_*^2\big(\frac{\pi}{2} - \sqrt{2\boldsymbol{\epsilon}} - \frac{t}{\tau}\big) \leq p_t \leq \sin_*^2\big(\frac{\pi}{2} - \sqrt{\frac{\boldsymbol{\epsilon}}{2} + \frac{t}{\tau}}\big), \tag{4.4}$$

where $\sin_*$ is defined by (5.5) *and τ is a positive constant given by*

$$\tau = \sqrt{2}\lambda_E^{-1/2} e^{(1-\varepsilon)\rho_A(V;e_N)}, \tag{4.5}$$

with $\lambda_E = C_E^2(V_0 + w)\lambda^4$.

Remark 4.3. In other words the result reads as follows: a state prepared at $t = 0$ in a state well localized in the potential well, does not escape from it with high probability p_t for any time t such that $t \ll \tau$. Namely as ϵ is small, the lower and upper bounds are near to 1 provided that the ratio $\frac{t}{\tau}$ is small.

Proof of Theorem 4.2. It relies on a generalized time-energy uncertainty relation due to Pfeifer and Fröhlich (see Proposition 5.1).

Let us consider the unitary groups $U_t := e^{-i\lambda t H}$ and $U_t^{(0)} := e^{-i\lambda t H_0}$ together with the projector $\bar{P}_t := U_t^{(0)^*} P_{\lambda,E} U_t^{(0)} \equiv P_{\lambda,E}$ and the conjugate dynamics

$$\bar{H}_t := U_t^{(0)^*}[H - i\lambda\partial_t]U_t^{(0)} = U_t^{(0)^*}(H - H_0)U_t^{(0)} = U_t^{(0)^*} W_\lambda U_t^{(0)}.$$

From Proposition 5.1 in the Appendix , taking $R = P_{\lambda,E} = P_{\lambda,E}^* = P_{\lambda,E}^2$ in (5.1), we obtain

$$f(\bar{P}_t, \bar{H}_s) = f\big(U_{t-s}^{(1)^*} P_{\lambda,E} U_{t-s}^{(1)}\ , W_\lambda\big) = f(P_{\lambda,E}, W_\lambda),$$

and using cyclicity of the trace in (5.1) we end with

$$f^2(P_{\lambda,E}, W_\lambda) = \frac{1}{2}\ \operatorname{tr}(-[P_{\lambda,E}\ , W_\lambda]^2). \tag{4.6}$$

Denoting by $K_{\lambda,E}(x,y)$ the kernel of the operator $P_{\lambda,E}$ in $L^2(X)$, we first observe after (4.3) that

$$\int_{X\times X} |K_{\lambda,E}(x,y)|^2 \Phi_E^2(x)\Phi_E^2(y)\, dV_g(x)\, dV_g(y) \leq C_E^2, \tag{4.7}$$

for a constant C_E. We compute the trace in (4.6) as follows

$$\begin{aligned}
&\frac{1}{2}\ \operatorname{tr}(-[P_{\lambda,E}\ , W_\lambda]^2)\\
&= \frac{1}{4}\int_{X\times X} |K_{\lambda,E}(x,y)[W_\lambda(x) - W_\lambda(y)]|^2 dV_g(x)\, dV_g(y)\\
&\leq \int_{X\times X} |K_{\lambda,E}(x,y)|^2 \Phi_E^2(x)\Phi_E^2(y) e^{-2(1-\varepsilon)(\rho_A(x;\widetilde{V},e_N) + \rho_A(y;\widetilde{V},e_N))}\\
&\quad \times [W_\lambda(x) - W_\lambda(y)]^2\, dV_g(x)\, dV_g(y).
\end{aligned} \tag{4.8}$$

Using (4.7) and (4.3) we can bound the integral in the right-hand side of (4.8) and we end with

$$\mathrm{tr}(-[P_{\lambda,E}\ ,W_\lambda]^2) \le \lambda_E e^{-2(1-\varepsilon)\rho_A(V,e_N)}, \tag{4.9}$$

for a positive constant $\lambda_E = C_E^2(V_0+w)^2\lambda^4$.

Defining now $\rho_t := U_t\rho_0 U_t^*$ and $p_t := \mathrm{tr}(\rho_t P_{\lambda,E})$, we are in position to apply the second result of Pfeifer and Fröhlich (see Propostion 5.2).

Let U_t and $U_t^{(1)}$ be the unitary groups defined above and given by

$$U_t := e^{-i\lambda tH}, \quad U_t^{(0)} := e^{-i\lambda tH_0},$$

together with the projector

$$\bar{P}_t := {U_t^{(0)}}^* P_{\lambda,E} U_t^{(0)} \equiv P_{\lambda,E}.$$

Consider the conjugate dynamics

$$\bar{H}_t := {U_t^{(0)}}^*[H - i\lambda\partial_t]U_t^{(0)} = {U_t^{(0)}}^*(H-H_0)U_t^{(0)}.$$

Then we have the bounds from above and from below for the probability p_t,

$$\begin{aligned}
&\sin_*^2\Big(\arcsin\sqrt{\mathrm{tr}(\bar{P}_{\lambda,E}\rho_0)} - \min\Big\{\int_0^t f(\bar{P}_{\lambda,E},\bar{H}_s)\,ds, \int_0^t f(\rho_0,\bar{H}_s)\,ds\Big\}\Big)\\
&\le p_t\\
&\le \sin_*^2\Big(\arcsin\sqrt{\mathrm{tr}(\bar{P}_{\lambda,E})\rho_0} + \min\Big\{\int_0^t f(\bar{P}_{\lambda,E},\bar{H}_s)\,ds, \int_0^t f(\rho_0,\bar{H}_s)\,ds\Big\}\Big),
\end{aligned}$$

where $f(R,A)$ is defined by (5.1) and the continuous function $\sin_*$ is defined by (5.5).

Supposing that we prepare the initial density according $\mathrm{tr}(\rho_0 P_{\lambda,E}) \ge (1-\boldsymbol{\epsilon})^2$ for a small $\boldsymbol{\epsilon} > 0$, we obtain the estimate

$$\begin{aligned}
&\sin_*^2\Big(\arcsin(1-\boldsymbol{\epsilon}) - \int_0^t f(P_{\lambda,E},\bar{H}_s)\,ds\Big)\\
&\le p_t \le \sin_*^2\Big(\arcsin(1-\boldsymbol{\epsilon}) + \int_0^t f(P_{\lambda,E},\bar{H}_s)\,ds\Big).
\end{aligned}$$

After (4.6) and (4.9) we see that $0 \le f(P_{\lambda,E},\bar{H}_s) \le \frac{\lambda_E^{1/2}}{\sqrt{2}} e^{-(1-\varepsilon)\rho_A(V,e_N)}$, and that $\frac{\pi}{2} - \sqrt{2\boldsymbol{\epsilon}} \le \arcsin(1-\varepsilon) \le \frac{\pi}{2} - \sqrt{\frac{\boldsymbol{\epsilon}}{2}}$, so we obtain (4.4) and we conclude that the density operator ρ_t of the system remains in the range of the projector $P_{\lambda,E}$ with probability p_t for all times $t \ll \tau$ where τ is given by (4.5). □

Remark 4.4. To recover formula (1.1), we observe that V and e_n are of order λ^2 so we see that $\rho_A(V,e_N) := \lambda(1-\varepsilon)b$ with (see 3.8)

$$\begin{aligned}
b := &\inf_{x\in S_V^-(E),y\in S_V^+(E)}\Big(\inf_{\{\gamma\in AC[0,1]:\gamma(0)=x,\gamma(1)=y\}}\int_0^1 \Big[\Big(\frac{V(\gamma(t))}{\lambda^2} - \frac{e_N}{\lambda^2}\Big)_+\Big]^{1/2}\\
&\times [g_{ij}(\gamma(t))\dot\gamma_i(t)\dot\gamma_j(t)]^{1/2}dt\Big).
\end{aligned}$$

Then the lifetime τ is as expected of the form (1.1) with computable constants $\lambda = \frac{1}{\hbar}$, $B = (1-\varepsilon)b$ and $A = \sqrt{2}\lambda_E^{-1/2}$.

5. Appendix: Uncertainty relations after Pfeifer and Fröhlich [27]

The first result is an uncertainty relation for subspaces and the second one is a generalized time-energy uncertainty relation. Both of them are proved in [27].

Proposition 5.1. *For a positive operator R with pure point spectrum with eigenvalues $\{\lambda_n\}_{n=1,\dots,N}$ and eigenprojectors $\{P_n\}_{n=1,\dots,N}$, and for two selfadjoint operators A and B, let us define the function f by*

$$f(R,A) = \Big(\sum_{n=1}^{N} \lambda_n \operatorname{tr}(P_n A^2 - P_n A P_n A)\Big)^{1/2}. \tag{5.1}$$

Then

$$|\operatorname{tr}(R[A,B])|^2 \le 4 f^2(R,A) f^2(R,B).$$

Proposition 5.2. *Let $U_{t,s}$ be the unitary group defining the evolution from time s to t for a system described by the (possibly t-dependent) Hamiltonian H_t, solution of the equation*

$$U_{t,s} = 1 - \frac{i}{\hbar}\int_s^t H_\tau U_{\tau,s}\, d\tau, \tag{5.2}$$

for all $s,t \in \mathbb{R}$. Let ρ_0 an initial density operator and P a projector. Define

$$\rho_{t,s} := U_{t,s}\rho_0 U_{t,s}^*, \quad p_{t,s} := \operatorname{tr}(P\rho_{t,s}). \tag{5.3}$$

Then we have the following bounds from above and from below for the probability $p_t = \operatorname{tr}(\rho_t P)$,

$$\begin{aligned} &\sin_*^2\Big(\arcsin\sqrt{\operatorname{tr}(P\rho_0)} - \hbar^{-1}\min\Big\{\int_s^t f(P,H_\tau)\,d\tau, \int_s^t f(\rho_0,H_\tau)\,d\tau\Big\}\Big)\\ &\le p_{t,s}\\ &\le \sin_*^2\Big(\arcsin\sqrt{\operatorname{tr}(P\rho_0)} + \hbar^{-1}\min\Big\{\int_s^t f(P,H_\tau)\,d\tau, \int_s^t f(\rho_0,H_\tau)\,d\tau\Big\}\Big), \end{aligned} \tag{5.4}$$

where f is defined for any A self-adjoint by $f(P,A) = \sqrt{\operatorname{tr}(PA^*(1-P)A)}$ and the continuous function $\sin_* : \mathbb{R} \to \mathbb{R}_+$ is given by

$$\sin_*(x) = \begin{cases} 0 & \text{if } x < 0,\\ \sin(x) & \text{if } 0 \le x \le \frac{\pi}{2},\\ 1 & \text{if } x > \frac{\pi}{2}. \end{cases} \tag{5.5}$$

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