Adiabatic analysis of the Landau Hamiltonian driven by a time-dependent Aharonov-Bohm flux*

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Abstract

We study the dynamics of a charged particle moving in a plane under the influence of a constant magnetic field and driven by a slowly time-dependent singular flux tube through a puncture. We discuss the meaning of the propagator and show that an adiabatic approximation is valid. To this end we develop the notion of a propagator weakly associated to a time-dependent Hamiltonian.

1 Introduction

The model under consideration originates from Laughlin's [13] and Halperin's [9] discussion of the Integer Quantum Hall effect. In the mathematical physics literature Bellissard [5] and Avron, Seiler, Simon [3] used an adiabatic limit of the model (with additional randomness) to introduce indices. The indices explain the quantization of charge transport observed in the experiments [12].

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In this paper we discuss some mathematical aspects of the existence of the propagator and the validity of the adiabatic approximation and propose how to overcome the difficulties originating from the strong singularity of the external field.

Let us specify the model, summarize our results and introduce the notation. The configuration space is $\mathbb{R}^2 \setminus \{(0,0)\}$ and the model is considered in polar coordinates (r, θ). The vector potential A is the sum of a part for the homogeneous magnetic field of strength $B > 0$,

$$\frac{B}{2}\,(x_1 \mathrm{d}x_2 - x_2 \mathrm{d}x_1) = \frac{Br^2}{2}\,\mathrm{d}\theta,$$

plus a part describing the flux Φ which varies in time,

$$\frac{\Phi}{2\pi}\,\frac{1}{|\vec{x}|^2}\,(x_1 \mathrm{d}x_2 - x_2 \mathrm{d}x_1) = \frac{\Phi}{2\pi}\,\mathrm{d}\theta;$$

the real-valued function Φ is assumed to be monotonous and C^2. With the metric coefficients $g_{11} = 1$, $g_{22} = r^2$, $g_{12} = 0$, the differential expression of the Hamiltonian acting in $L^2(\mathbb{R}_+ \times [0, 2\pi[\,, r\mathrm{d}r\mathrm{d}\theta)$ is

$$\begin{aligned}
&\frac{1}{2m}\left(-i\hbar\partial_j - \frac{e}{c}A_j\right)\sqrt{g}g^{jk}\left(-i\hbar\partial_k - \frac{e}{c}A_k\right)\\
&= \frac{\hbar^2}{2m}\left(-\frac{1}{r}\partial_r r\partial_r + \frac{1}{r^2}\left(-i\partial_\theta - \frac{e}{\hbar c}\frac{Br^2}{2} - \frac{e}{hc}\,\Phi\right)^2\right).
\end{aligned}$$

Our purpose is to study the response of the system if flux quanta hc/e are added adiabatically, i.e. the flux function is of the form $t \mapsto \Phi(t/\tau)$ with the time t varying in $[\,0, \tau\,]$ for some $\tau \gg 1$.

In a first step we analyze the case when Φ is linear. Furthermore, we fix an angular momentum sector defined by $-i\partial_\theta e^{im\theta} = me^{im\theta}$ ($m \in \mathbb{Z}$), and use a slow time s, i.e.: the substitution $s = -m + e/(hc)\Phi(t/\tau)$. Also we are not interested here in keeping track of the behavior in the physical parameters e, $\hbar$, c, $2m$, so we set them all equal to one. This is our motivation to consider the operator

$$H(s) = -\frac{1}{r}\partial_r r\partial_r + \frac{1}{r^2}\left(s + \frac{Br^2}{2}\right)^2 \quad \text{in } L^2(\mathbb{R}_+, r\mathrm{d}r). \tag{1}$$

In a second step we shall then show that our analysis generalizes to Hamiltonians of the form $H\big(\zeta(s)\big)$ where $\zeta \in C^2$ is a monotone function.

$H(s)$ is essentially selfadjoint on $C_0^\infty(]0, \infty[)$ iff $s^2 \geq 1$ [14]. For $0 < s^2 < 1$ we impose the regular boundary condition as $r \to 0+$ (i.e.: a wavefunction belongs to the domain if it has no part proportional to the (square integrable) singularity $r^{-|s|}$). This is in fact the most common choice, see [8] for a detailed discussion. The case $s = 0$ is particular since the singularity in question is logarithmic but otherwise the situation is similar, see [1]. The Hamiltonian $H(s)$ is unambiguously determined by specifying a complete set of eigenfunctions with corresponding eigenvalues, see below.

The dynamics of the model should be defined by

$$i\partial_s U_\tau(s, s_0)\psi = \tau H(s) U_\tau(s, s_0)\psi, \quad U_\tau(s_0, s_0)\psi = \psi, \tag{2}$$

where U_τ is unitary and ψ is an arbitrary initial condition from the domain of $H(s_0)$. The existence of a propagator in this sense is, however, uncertain. The problem arises from the fact that the domain of $H(s)$ is not constant in s, respectively that $\dot{H}(s)$ is not relatively bounded with respect to $H(s)$. Thus the usual theorems which assure the existence of the propagator [14] and the validity of the adiabatic approximation [4, 2] are not directly applicable.

A convenient way to see this is to consider the eigenfunctions. The operator $H(s)$ has a simple discrete spectrum; the eigenvalues are

$$\lambda_n(s) = B(s + |s| + 2n + 1), \qquad n \in \{0, 1, 2, \ldots\}, \tag{3}$$

with the corresponding normalized eigenfunctions

$$\varphi_n(s; r) = c_n(s)\, r^{|s|}\, L_n^{(|s|)}\left(\frac{Br^2}{2}\right) \exp\left(-\frac{Br^2}{4}\right)$$

where

$$c_n(s) = \left(\frac{B}{2}\right)^{(|s|+1)/2} \left(\frac{2\, n!}{\Gamma(n + |s| + 1)}\right)^{1/2}$$

are the normalization constants and $L_n^{(|s|)}$ are the generalized Laguerre polynomials (see, for example, [8]).

The derivative of $H(s)$ equals

$$\dot{H}(s) = \frac{2s}{r^2} + B.$$

Notice that if $|s| \leq 1$ then $\varphi_n(s)$ cannot belong to the domain $\operatorname{Dom} \dot{H}(s)$ since $\dot{H}(s)\varphi_n(s) \sim r^{-2+|s|}$ for $r \to 0+$. This means that $\dot{H}(s)$ is not relatively bounded with respect to $H(s)$.

Remark that, on the other hand, the quadratic expression

$$\int_0^\infty \varphi_m(s; r)\, \dot{H}(s) \varphi_n(s; r)\, r \, \mathrm{d}r$$

makes good sense. In order to avoid a complicated notation we shall denote it by the symbol $\langle \varphi_m(s), \dot{H}(s)\varphi_n(s)\rangle$ even though the symbol cannot be taken literally and is therefore somewhat misleading. Furthermore, the derivative of the eigenfunction, $\dot{\varphi}_n(s)$, belongs to $L^2(\mathbb{R}_+, r\,\mathrm{d}r)$. Since the eigenfunctions are chosen to be real-valued it holds true that

$$\langle \varphi_n(s), \dot{\varphi}_n(s)\rangle = 0.$$

Let us also note that, similarly, if $|s| \leq 1$ and $s^2 \neq s'^2$ then the eigenfunction $\varphi_n(s)$ cannot belong to $\mathrm{Dom}\, H(s')$. It is so because (as formal expressions) $H(s') - H(s) = (s'^2 - s^2)/r^2 + B(s' - s)$ and $H(s')\varphi_n(s;r)$ has a non-integrable singularity at $r = 0$. Hence $\mathrm{Dom}\, H(s)$ depends on s.

It turns out that, following the strategy of Born and Fock [7], the problems of existence and adiabatic approximation can both be handled:

denote the eigenprojector onto $\mathbb{C}\varphi_n(s)$ by $P_n(s)$; it is differentiable as a bounded operator. The hard part of our work consists in showing that

$$i\sum_{k=0}^{\infty} \dot{P}_k(s)P_k(s)$$

is a bounded operator. This is stated in Lemma 6. It requires work because its matrix elements have bad off–diagonal decay, see Lemma 4 (which is formulated for the unitarily equivalent operator Q).

Now

$$H_{AD}(s) := H(s) + \frac{i}{\tau}\sum_{n=0}^{\infty} \dot{P}_n(s)P_n(s)$$

has a propagator which is well defined in the usual way, i.e.

$$i\partial_s U_{AD}(s,s_0)\psi = \tau H_{AD}(s)U_{AD}(s,s_0)\psi, \quad U_{AD}(s_0,s_0)\psi = \psi, \tag{4}$$

for $\psi \in \mathrm{Dom}\,(H_{AD}(s_0))$. To see this notice that U_{AD} can be computed by its action on the eigenbasis:

$$U_{AD}(s,s_0)\varphi_n(s_0) = e^{-i\tau\int_{s_0}^{s}\lambda_n(u)\,\mathrm{d}u}\varphi_n(s).$$

Furthermore, $\lambda_n(s) - \lambda_n(0)$ is bounded in n and so $U_{AD}(s,s_0)\,\mathrm{Dom}\, H_{AD}(s_0) = \mathrm{Dom}\, H_{AD}(s)$.

Since $H(s) - H_{AD}(s)$ is bounded the domains of $H(s)$ and $H_{AD}(s)$ are identical. By time-dependent transformation a natural candidate for the propagator of $H(s)$ is

$$U_\tau(s,s_0) := U_{AD}(s,0)C(s,s_0)U_{AD}(0,s_0) \tag{5}$$

where $C(s, s_0)$ is defined by

$$i\partial_s C(s, s_0) = -Q_\tau(s) C(s, s_0), \quad C(s_0, s_0) = \mathbb{I}, \tag{6}$$

with

$$Q_\tau(s) := U_{AD}(0, s) \left(i \sum_{k=0}^{\infty} \dot{P}_k(s) P_k(s) \right) U_{AD}(s, 0). \tag{7}$$

Since $\|Q_\tau(s)\|$ is locally bounded the propagator $C(s, s_0)$ is well defined by the Dyson formula.

The adiabatic approximation problem is settled in Proposition 11 were it is shown that

$$\|U_\tau(s, 0) - U_{AD}(s, 0)\| = O\left(\frac{1}{\tau}\right).$$

It remains unclear, however, whether $C(s, s_0)$ preserves the domain of $H(0)$ and therefore whether the propagator $U_\tau(s, s_0)$ is actually related to the Hamiltonian $H(s)$ in the usual sense. To handle this problem we develop the general concept of weak association of a propagator and a time dependent Hamiltonian. We can show that U_τ is weakly associated to $H(s)$ and that the Schrödinger equation (2) is fulfilled in the sense of distributions.

We shall use the following notation. The symbol $V(s)$ stands for the unitary operator which sends all eigenstates at time 0 to the corresponding eigenstates at time s, i.e.

$$V(s)\varphi_n(0) = \varphi_n(s) \qquad \forall n \in \mathbb{Z}_+ \tag{8}$$

(here and everywhere in what follows $\mathbb{Z}_+$ stands for the set of nonnegative integers). Further set

$$W(s) = V(s)^{-1} H(s) V(s) = \sum_{n=0}^{\infty} \lambda_n(s)\, P_n(0) \tag{9}$$

and

$$\Omega(s) = \sum_{n=0}^{\infty} \omega_n(s)\, P_n(0) \tag{10}$$

where

$$\omega_n(s) = \int_0^s \lambda_n(u)\, \mathrm{d}u.$$

Remark that the adiabatic propagator decomposes as

$$U_{AD}(s, s_0) = V(s) e^{-i\tau(\Omega(s) - \Omega(s_0))} V(s_0)^{-1}.$$

The paper is organized as follows. In Sections 2 and 3 we do the analysis necessary to prove the boundedness result stated in Lemma 6. Section 4 is devoted to the existence problem for the propagator. In Section 5 we prove the adiabatic theorem in Proposition 11. The result is then extended to a more general time-dependence in Section 6.

A rather independent part of the paper is the Appendix where we propose the notion of a propagator weakly associated to a time-dependent Hamiltonian. We indicate cases where the weak association can be verified while the usual relationship between a propagator and a Hamiltonian is unclear or even is not valid. In particular, this concept was inspired by the situation we encountered in the present model. We believe, however, that this idea need not be restricted to this case only and that it might turn out to be useful in resolving this type of difficulties in other models as well.

2 Auxiliary estimates of matrix operators

Here we derive some auxiliary estimates that will be useful later when verifying assumptions of the adiabatic theorem.

Lemma 1. *Let $A(\sigma)$ be an operator in $l^2(\mathbb{N})$ depending on a parameter $\sigma \geq 0$ whose matrix entries in the standard basis equal*

$$A(\sigma)_{mn} = \begin{cases} 0 & \text{for } m = n \\ -\frac{i}{n}\left(\frac{m}{n}\right)^{\sigma} & \text{for } m < n \\ \frac{i}{m}\left(\frac{n}{m}\right)^{\sigma} & \text{for } m > n \end{cases}.$$

Then $A(\sigma)$ is bounded, uniformly in σ, and its norm satisfies the estimate

$$\|A(\sigma)\| \leq 24.$$

Proof. The proof will be done in several steps.

(i) Let $K(\sigma)$ be an integral operator acting in $L^2(\mathbb{R}_+, \mathrm{d}x)$ with the integral kernel

$$\mathcal{K}_\sigma(x,y) = \begin{cases} -\frac{i}{y}\left(\frac{x}{y}\right)^{\sigma} & \text{for } x < y \\ \frac{i}{x}\left(\frac{y}{x}\right)^{\sigma} & \text{for } x > y \end{cases}.$$

Let us show that

$$\|K(\sigma)\| = \frac{2}{2\sigma+1}\,.$$

First we apply the unitary transform

$$U : L^2(\mathbb{R}_+, \mathrm{d}x) \to L^2(\mathbb{R}, \mathrm{d}y),\ U\psi(y) = e^{y/2}\psi(e^y). \tag{11}$$

The inverse transform reads $U^{-1}\hat{\psi}(x) = x^{-1/2}\hat{\psi}(\ln x)$. Set

$$\tilde{K}(\sigma) = UK(\sigma)U^{-1}.$$

One finds that $\tilde{K}(\sigma)$ is again an integral operator with the integral kernel

$$\tilde{\mathcal{K}}_\sigma(y,z) = i\,\mathrm{sgn}(y-z)\,e^{-(\sigma+1/2)|y-z|}.$$

Hence $\tilde{K}(\sigma)$ is a convolution operator and it is therefore diagonalizable with the aid of the Fourier transform $\mathcal{F}$ on $\mathbb{R}$. This means that

$$\big(\mathcal{F}\tilde{K}(\sigma)\mathcal{F}^{-1}\psi\big)(z) = \hat{q}(z)\psi(z)$$

where

$$\hat{q}(z) = \int_{\mathbb{R}} e^{izy}\,\mathrm{sgn}(y)\,e^{-(\sigma+1/2)|y|}\,\mathrm{d}y = \frac{2iz}{\left(\sigma+\frac{1}{2}\right)^2 + z^2}\,.$$

It follows that

$$\|K(\sigma)\| = \|\mathcal{F}\tilde{K}(\sigma)\mathcal{F}^{-1}\| = \|\hat{q}\|_\infty = \frac{1}{\sigma+\frac{1}{2}}\,. \tag{12}$$

(ii) Suppose that $\{\psi\}_{n=1}^\infty$ is an orthogonal system in $L^2(\mathbb{R}_+,\mathrm{d}x)$ such that

$$\forall m,n\in\mathbb{N},\ \langle\psi_m, K(\sigma)\psi_n\rangle = A(\sigma)_{mn}$$

and

$$\forall n\in\mathbb{N},\ \|\psi_n\|^2 = \kappa > 0.$$

Let P_+ be the orthogonal projector onto $\mathrm{span}\{\psi_n\}_{n=1}^\infty$ in $L^2(\mathbb{R}_+,\mathrm{d}x)$. Then one can identify $P_+K(\sigma)P_+$ with $\kappa^{-1}A(\sigma)$. Hence

$$\|A(\sigma)\| = \kappa\|P_+K(\sigma)P_+\| \leq \kappa\|K(\sigma)\|. \tag{13}$$

(iii) We shall construct an orthogonal system $\{\psi_n\}_{n=1}^\infty$ described in the preceding point as follows. Consider the natural embedding $L^2([n,n+1],\mathrm{d}x) \subset L^2(\mathbb{R}_+,\mathrm{d}x)$, $n\in\mathbb{N}$. We seek $\psi_n \in L^2([n,n+1],\mathrm{d}x)$ in the form

$$\psi_n = \alpha_n u_n + \beta_n v_n + f_n$$

where $\alpha_n,\beta_n\in\mathbb{R}$, $u_n, v_n, f_n \in L^2([n,n+1],\mathrm{d}x)$,

$$u_n(x) = x^\sigma,\ v_n(x) = x^{-\sigma-1} \text{ for } x\in[n,n+1],$$

and $f_n \perp u_n$, $f_n\perp v_n$. Suppose for definiteness that $m<n$. Then

$$\begin{aligned}\langle\psi_m, K(\sigma)\psi_n\rangle &= \int_m^{m+1}\mathrm{d}x\int_n^{n+1}\mathrm{d}y\,\mathcal{K}_\sigma(x,y)\,\psi_m(x)\,\psi_n(y)\\ &= -i\,\langle u_m,\psi_m\rangle\,\langle v_n,\psi_n\rangle\,.\end{aligned}$$

Furthermore,

$$\langle \psi_n, K(\sigma)\psi_n \rangle = \int_n^{n+1} \int_n^{n+1} \mathcal{K}_\sigma(x,y)\,\psi_n(x)\,\psi_n(y)\,\mathrm{d}x\mathrm{d}y = 0$$

since $\mathcal{K}_\sigma(x,y)$ is antisymmetric, $\mathcal{K}_\sigma(y,x) = -\mathcal{K}_\sigma(x,y)$. Consequently, it suffices to choose the real coefficients α_n, β_n so that

$$\forall n \in \mathbb{N},\ \langle u_n, \psi_n \rangle = n^\sigma,\ \langle v_n, \psi_n \rangle = n^{-\sigma-1}.$$

This system has a unique solution (α_n, β_n). The function f_n can be arbitrary. Its only purpose is to adjust the norms of the functions ψ_n so that they are all equal. Set

$$N_n(\sigma) = \|\alpha_n u_n + \beta_n v_n\|^2 = \int_n^{n+1} \left(\alpha_n x^\sigma + \beta_n x^{-\sigma-1}\right)^2 \mathrm{d}x$$

and

$$\kappa(\sigma) = \sup_{n\in\mathbb{N}} N_n(\sigma).$$

One can choose the orthogonal system $\{\psi_n\}_{n=1}^\infty$ so that $\|\psi_n\|^2 = \kappa(\sigma)$ for all n. According to (12) and (13) we have

$$\|A(\sigma)\| \le \frac{2\,\kappa(\sigma)}{2\sigma+1}\,. \tag{14}$$

(iv) It remains to find an upper bound on $\kappa(\sigma)$. Set

$$\xi_n = n^\sigma,\ \eta_n = n^{-\sigma-1}.$$

Simple algebraic manipulations yield

$$N_n(\sigma) = \frac{\langle v_n, v_n\rangle\,\xi_n^2 - 2\,\langle u_n, v_n\rangle\,\xi_n\eta_n + \langle u_n, u_n\rangle\,\eta_n^2}{\langle u_n, u_n\rangle\,\langle v_n, v_n\rangle - \langle u_n, v_n\rangle^2}\,.$$

Here

$$\begin{aligned}
\langle u_n, v_n\rangle &= \ln\!\left(1+\frac{1}{n}\right),\\
\langle u_n, u_n\rangle &= \frac{1}{2\sigma+1}\left((n+1)^{2\sigma+1} - n^{2\sigma+1}\right),\\
\langle v_n, v_n\rangle &= \frac{1}{2\sigma+1}\left(n^{-2\sigma-1} - (n+1)^{-2\sigma-1}\right).
\end{aligned}$$

Set

$$w = \left(\sigma+\frac{1}{2}\right)\ln\!\left(1+\frac{1}{n}\right).$$

One can rewrite the expression for $N_n(\sigma)$ as follows,

$$N_n(\sigma) = \frac{2\sigma+1}{n}\,\frac{\sinh(w)\cosh(w)-w}{\sinh^2(w)-w^2}\,.$$

Using an elementary analysis one can show that

$$\frac{\sinh(w)\cosh(w)-w}{\sinh^2(w)-w^2} \leq \frac{\sinh(w)\cosh(w)-w}{\sinh(w)\,(\sinh(w)-w)} \leq 4\,\mathrm{cotgh}(w).$$

Hence

$$N_n(\sigma) \leq \frac{4(2\sigma+1)}{n}\,\frac{\left(1+\frac{1}{n}\right)^{2\sigma+1}+1}{\left(1+\frac{1}{n}\right)^{2\sigma+1}-1} \leq 12(2\sigma+1).$$

Consequently,

$$\kappa(\sigma) \leq 12(2\sigma+1). \tag{15}$$

From (14) and (15) it follows that $\|A(\sigma)\| \leq 24$. □

Lemma 2. *Let $A(\sigma)$ be an operator in $l^2(\mathbb{N})$ whose matrix entries in the standard basis equal*

$$A(\sigma)_{mn} = \begin{cases} 0 & \text{for } m=n \\ -\frac{i}{n}\,f_\sigma\!\left(\frac{m}{n}\right) & \text{for } m<n \\ \frac{i}{m}\,f_\sigma\!\left(\frac{n}{m}\right) & \text{for } m>n \end{cases}$$

where

$$f_\sigma(u) = \frac{1-u^\sigma}{1-u}\,,\ \ u \in\,]0,1[\,,$$

and $\sigma \in [0,1]$ is a parameter. Then $A(\sigma)$ is bounded and its norm satisfies the estimate

$$\|A(\sigma)\| \leq \left(\frac{\sqrt{2}}{3}+4\right)\pi^2\sigma.$$

Proof. The proof will be done in several steps.

(i) Let $K(\sigma)$ be an integral operator acting in $L^2(\mathbb{R}_+,\mathrm{d}x)$ with the integral kernel

$$\mathcal{K}_\sigma(x,y) = \begin{cases} -\frac{i}{y}\,f_\sigma\!\left(\frac{x}{y}\right) & \text{for } x<y \\ \frac{i}{x}\,f_\sigma\!\left(\frac{y}{x}\right) & \text{for } x>y \end{cases}.$$

Let us show that

$$\|K(\sigma)\| \leq \pi^2\sigma. \tag{16}$$

This step is quite analogous to the proof of point (i) in Lemma 1. First we apply the unitary transform U defined in (11). Set

$$\tilde{K}(\sigma) = UK(\sigma)U^{-1}.$$

One finds that $\tilde{K}(\sigma)$ is again an integral operator with the integral kernel

$$\tilde{\mathcal{K}}_\sigma(y,z) = i\,\mathrm{sgn}(y-z)\,f_\sigma\big(e^{-|y-z|}\big)\,e^{-|y-z|/2}.$$

Thus $\tilde{K}(\sigma)$ is a convolution operator which is diagonalizable with the aid of the Fourier transform $\mathcal{F}$ on $\mathbb{R}$. This means that $\big(\mathcal{F}\tilde{K}(\sigma)\mathcal{F}^{-1}\psi\big)(z) = \hat{q}(z)\psi(z)$ where

$$\hat{q}(z) = \int_{\mathbb{R}} e^{izy}\,\mathrm{sgn}(y)\,f_\sigma\big(e^{-|y|}\big)\,e^{-|y|/2}\,\mathrm{d}y.$$

A standard estimate yields

$$|\hat{q}(z)| \leq 2\int_0^\infty \frac{1-e^{-\sigma y}}{1-e^{-y}}\,e^{-y/2}\,\mathrm{d}y \leq \sigma\int_0^\infty \frac{y}{\sinh(y/2)}\,\mathrm{d}y = \pi^2\sigma.$$

It follows that

$$\|K(\sigma)\| = \|\mathcal{F}\tilde{K}(\sigma)\mathcal{F}^{-1}\| = \|\hat{q}\|_\infty \leq \pi^2\sigma.$$

(ii) Let $\chi_n(x)$ be the characteristic function of the interval $]n,n+1[$. The linear mapping

$$J : l^2(\mathbb{N}) \to L^2(\mathbb{R}_+,\mathrm{d}x) : \{\xi_n\} \mapsto \sum_{n=1}^\infty \xi_n\chi_n$$

is an isometry. The adjoint mapping reads

$$J^* : L^2(\mathbb{R}_+,\mathrm{d}x) \to l^2(\mathbb{N}) : \psi \mapsto \{\langle\chi_n,\psi\rangle\}_{n=1}^\infty.$$

Set

$$L(\sigma) = JA(\sigma)J^*.$$

$L(\sigma)$ is an integral operator with the kernel

$$\mathcal{L}_\sigma(x,y) = \sum_{m=1}^\infty\sum_{n=1}^\infty A(\sigma)_{mn}\chi_m(x)\chi_n(y).$$

This can be rewritten as

$$\mathcal{L}_\sigma(x,y)=\begin{cases}-\frac{i}{[y]}\,f_\sigma\left(\frac{[x]}{[y]}\right) & \text{if } 0<[x]<[y]\\ \frac{i}{[x]}\,f_\sigma\left(\frac{[y]}{[x]}\right) & \text{if } 0<[y]<[x]\\ 0 & \text{otherwise}\end{cases}.$$

Here $[x]$ denotes the integer part of x. Notice that J^*J is the identity on $l^2(\mathbb{N})$ and so $L(\sigma)J=JA(\sigma)$. Consequently,

$$\|A(\sigma)\|=\|JA(\sigma)\|=\|L(\sigma)J\|\le\|L(\sigma)\|. \tag{17}$$

(iii) Denote by $\tilde{P}_n$, $n\in\mathbb{Z}_+$, the orthogonal projector onto $\mathbb{C}\chi_n$ in $L^2(\mathbb{R}_+,\mathrm{d}x)$. Set

$$K^{\mathrm{off}}(\sigma)=K(\sigma)-\tilde{P}_0K(\sigma)-K(\sigma)\tilde{P}_0+\tilde{P}_0K(\sigma)\tilde{P}_0-\sum_{n=1}^{\infty}\tilde{P}_nK(\sigma)\tilde{P}_n.$$

In other words, we subtract from $K(\sigma)$ the diagonal as well as the first row and the first column (i.e., with index 0) with respect to the orthogonal system $\{\chi_n\}_{n=0}^{\infty}$. We can say also that the integral kernel $\mathcal{K}_\sigma^{\mathrm{off}}(x,y)$ vanishes if $[x]=[y]$ or $[x]=0$ or $[y]=0$ and otherwise it coincides with $\mathcal{K}_\sigma(x,y)$. Since

$$\left\|\tilde{P}_0K(\sigma)\tilde{P}_0-\sum_{n=1}^{\infty}\tilde{P}_nK(\sigma)\tilde{P}_n\right\|=\sup_{n\in\mathbb{Z}_+}\|\tilde{P}_nK(\sigma)\tilde{P}_n\|\le\|K(\sigma)\|$$

we have

$$\|K^{\mathrm{off}}(\sigma)\|\le 4\|K(\sigma)\|. \tag{18}$$

(iv) It remains to estimate the norm of the difference $L(\sigma)-K^{\mathrm{off}}(\sigma)$. This is a Hermitian integral operator whose kernel does not vanish only if $0<[x]<[y]$ or $0<[y]<[x]$. Suppose for definiteness that $0<[x]<[y]$. Then the kernel equals, up to the multiplier $-i$,

$$\begin{aligned}\frac{1}{[y]}\,f_\sigma\left(\frac{[x]}{[y]}\right)-\frac{1}{y}\,f_\sigma\left(\frac{x}{y}\right) &= \left(\frac{1}{[y]^\sigma}-\frac{1}{y^\sigma}\right)\frac{[y]^\sigma-[x]^\sigma}{[y]-[x]}\\ &\quad+\frac{1}{y^\sigma}\left(\frac{[y]^\sigma-[x]^\sigma}{[y]-[x]}-\frac{y^\sigma-x^\sigma}{y-x}\right).\end{aligned}$$

Let us show that

$$0\le\frac{1}{[y]}\,f_\sigma\left(\frac{[x]}{[y]}\right)-\frac{1}{y}\,f_\sigma\left(\frac{x}{y}\right)\le\frac{2\sigma}{[x]([y]-[x])}. \tag{19}$$

First notice that

$$0 \le \frac{1}{[y]^\sigma} - \frac{1}{y^\sigma} = -\sigma \int_y^{[y]} z^{-\sigma-1} \mathrm{d}z \le \frac{\sigma(y-[y])}{[y]^{\sigma+1}}$$

and so

$$0 \le \left(\frac{1}{[y]^\sigma} - \frac{1}{y^\sigma} \right) \frac{[y]^\sigma - [x]^\sigma}{[y]-[x]} \le \frac{\sigma}{[y]([y]-[x])} \,. \tag{20}$$

Further set temporarily

$$\begin{aligned} D &= \frac{[y]^\sigma - [x]^\sigma}{[y]-[x]} - \frac{y^\sigma - x^\sigma}{y-x} \\ &= \sigma \int_0^1 \left(([x](1-t)+[y]t)^{\sigma-1} - (x(1-t)+yt)^{\sigma-1} \right) \mathrm{d}t \,. \end{aligned}$$

The integrand in the last integral equals

$$\sigma(1-\sigma)\xi_t^{\sigma-2} \left((x-[x])(1-t) + (y-[y])t \right)$$

where ξ_t is a real number lying between $[x](1-t)+[y]t$ and $x(1-t)+yt$. Notice that

$$0 \le (x-[x])(1-t) + (y-[y])t \le 1.$$

We assume that $0 \le \sigma \le 1$. Therefore

$$0 \le D \le \sigma(1-\sigma) \int_0^1 ([x](1-t)+[y]t)^{\sigma-2} \, \mathrm{d}t = -\sigma \, \frac{[y]^{\sigma-1} - [x]^{\sigma-1}}{[y]-[x]}$$

and so

$$0 \le \frac{1}{y^\sigma} D \le \frac{\sigma [x]^{\sigma-1}}{y^\sigma([y]-[x])} \le \frac{\sigma}{[x]([y]-[x])} \,. \tag{21}$$

Inequalities (20) and (21) jointly imply (19).

(v) From estimate (19) one can deduce that $L(\sigma) - K^{\mathrm{off}}(\sigma)$ is a Hilbert-Schmidt operator and

$$\|L(\sigma) - K^{\mathrm{off}}(\sigma)\|_{\mathrm{HS}} \le \frac{\sqrt{2}\,\pi^2}{3}\,\sigma. \tag{22}$$

Actually,

$$\begin{aligned} \|L(\sigma) - K^{\mathrm{off}}(\sigma)\|_{\mathrm{HS}}^2 &= 2 \int_1^\infty \mathrm{d}x \int_{[x]+1}^\infty \mathrm{d}y \left| \mathcal{L}_\sigma(x,y) - \mathcal{K}_\sigma^{\mathrm{off}}(x,y) \right|^2 \\ &\le 8\sigma^2 \int_1^\infty \mathrm{d}x \, \frac{1}{[x]^2} \int_{[x]+1}^\infty \mathrm{d}y \, \frac{1}{([y]-[x])^2} \\ &= 8\sigma^2 \left(\sum_{k=1}^\infty \frac{1}{k^2} \right)^2 . \end{aligned}$$

(vi) Inequalities (17), (18), (16) and (22) imply that

$$\|A(\sigma)\| \le \|L(\sigma)\| \le \|K^{\mathrm{off}}(\sigma)\| + \|L(\sigma) - K^{\mathrm{off}}(\sigma)\| \le 4\pi^2\sigma + \frac{\sqrt{2}\,\pi^2}{3}\,\sigma.$$

This shows the lemma. $\square$

Lemma 3. *Let $A(\sigma)$ be an operator in $l^2(\mathbb{N})$ with the matrix entries in the standard basis*

$$A(\sigma)_{mn} = \begin{cases} 0 & \text{for } m = n \\ \frac{i}{n-m}\,\min\{\left(\frac{m}{n}\right)^\sigma, \left(\frac{n}{m}\right)^\sigma\} & \text{for } m \neq n \end{cases}.$$

Then $A(\sigma)$ is bounded for all $0 \le \sigma$ and its norm satisfies the estimate

$$\|A(\sigma)\| \le \pi + \left(\frac{\sqrt{2}}{3} + 4\right)\pi^2\sigma.$$

Proof. Let us first show that

$$\|A(0)\| \le \pi.$$

For $\sigma = 0$ we get

$$A(0)_{mn} = \frac{i}{n-m} \quad \text{if } m \neq n.$$

Considering the natural embedding $l^2(\mathbb{N}) \subset l^2(\mathbb{Z})$ let us denote by P_+ the orthogonal projector onto $l^2(\mathbb{N})$ in $l^2(\mathbb{Z})$. Let B be an operator in $l^2(\mathbb{Z})$ with the matrix

$$B_{mn} = q(n-m) \text{ where } q(n) = \begin{cases} 0 & \text{for } n = 0 \\ \frac{i}{n} & \text{for } n \neq 0 \end{cases}.$$

One can identify $A(0)$ with P_+BP_+. B is a convolution operator and therefore it is diagonalizable by the Fourier transform $\mathcal{F} : l^2(\mathbb{Z}) \to L^2([0,2\pi], \mathrm{d}\theta)$. In more detail,

$$\left(\mathcal{F}B\mathcal{F}^{-1}\psi\right)(\theta) = \hat{q}(\theta)\psi(\theta) \text{ where } \hat{q}(\theta) = \sum_{n\in\mathbb{Z}} q(n)\,e^{in\theta}.$$

One finds that $\hat{q}(\theta) = -\pi + \theta$. Consequently,

$$\|A(0)\| = \|P_+BP_+\| \le \|B\| = \|\mathcal{F}B\mathcal{F}^{-1}\| = \max_{\theta\in[0,2\pi]} |\hat{q}(\theta)| = \pi.$$

Suppose now that $0 < m < n$. Notice that

$$(A(\sigma+1) - A(\sigma))_{mn} = -\frac{i}{n}\left(\frac{m}{n}\right)^{\sigma}$$

and

$$(A(\sigma) - A(0))_{mn} = -\frac{i}{n} f_\sigma\left(\frac{m}{n}\right).$$

Using Lemma 1 and Lemma 2 one can estimate

$$\begin{aligned}
\|A(\sigma)\| &\leq \|A(0)\| + \|A(\sigma - [\sigma]) - A(0)\| + \|A(\sigma - [\sigma] + 1) - A(\sigma - [\sigma])\| \\
&\quad + \ldots + \|A(\sigma) - A(\sigma - 1)\| \\
&\leq \pi + \left(\frac{\sqrt{2}}{3} + 4\right)\pi^2(\sigma - [\sigma]) + 24[\sigma] \\
&\leq \pi + \left(\frac{\sqrt{2}}{3} + 4\right)\pi^2\sigma.
\end{aligned}$$

This proves the lemma. □

3 Boundedness of the operator $i\sum_{k=0}^{\infty}\dot{P}_k(s)P_k(s)$

We consider $i\sum_{k=0}^{\infty}\dot{P}_k(s)P_k(s)$ in the time independent frame, i.e. the operator $Q(s)$ defined by

$$Q(s) = iV(s)^*\sum_{k=0}^{\infty}\dot{P}_k(s)P_k(s)V(s) = -i\dot{V}(s)^*V(s) = iV(s)^*\dot{V}(s). \tag{23}$$

The operator $V(s)$ is defined in (8). $Q(s)$ is symmetric and its matrix entries in the basis $\{\varphi_n(0)\}$ are

$$\langle\varphi_m(0), Q(s)\varphi_n(0)\rangle = i\,\langle\varphi_m(s), \dot{\varphi}_n(s)\rangle\,.$$

Since $\varphi_n(s)$ depends on s only through the absolute value it holds true that $Q(-s) = -Q(s)$ for $s \neq 0$. For $s = 0$ the operator-valued function $Q(s)$ has a discontinuity. The goal of this section is to show that the operator $Q(s)$ is in fact bounded.

To compute the matrix entries one can use the identity

$$\langle\varphi_m(s), \dot{\varphi}_n(s)\rangle = \frac{\left\langle\varphi_m(s), \dot{H}(s)\varphi_n(s)\right\rangle}{\lambda_n(s) - \lambda_m(s)}\,. \tag{24}$$

Let us emphasize once more that the scalar product on the RHS should be interpreted as a quadratic form since, in general, $\varphi_n(s) \notin \operatorname{Dom} \dot{H}(s)$. The derivation goes through basically as usual even though one cannot use the scalar product directly. Differentiating the equation on eigenvalues one arrives at the equality

$$H(s)\dot{\varphi}_n(s;r) + \dot{H}(s)\varphi_n(s;r) = \dot{\lambda}_n(s)\varphi_n(s;r) + \lambda_n(s)\dot{\varphi}_n(s;r),$$

valid for any $r > 0$, in which one should substitute for $H(s)$ and $\dot{H}(s)$ the corresponding formal differential operators. Next one multiplies the equality by $r\varphi_m(s;r)$ and integrates the both sides from ε to infinity for some $\varepsilon > 0$. In the integral

$$-\int_{\varepsilon}^{\infty} \varphi_m(s;r)\partial_r r \partial_r \dot{\varphi}_n(s;r)\,\mathrm{d}r$$

occurring on the LHS side one integrates twice by parts. Checking the asymptotic behavior of the eigenfunctions near the origin,

$$\varphi_n(s;r) \sim \left(\frac{B}{2}\right)^{(|s|+1)/2} \left(\frac{2\,n!}{\Gamma(n+|s|+1)}\right)^{1/2} r^{|s|}\left(1 + O(r^2)\right) \quad \text{for } r \to 0+, \tag{25}$$

one finds that

$$\lim_{r\to 0+} r\varphi_m(s;r)\partial_r\dot{\varphi}_n(s;r) = \lim_{r\to 0+} r\left(\partial_r\varphi_m(s;r)\right)\dot{\varphi}_n(s;r) = 0.$$

Hence sending ε to 0 actually leads to equality (24).

Lemma 4. *The matrix entries of the operator $Q(s)$ for $s \neq 0$ are given by the formulae*

$$\langle\varphi_m(0), Q(s)\varphi_n(0)\rangle = 0 \quad \textit{for } m = n,$$

and

$$\langle\varphi_m(0), Q(s)\varphi_n(0)\rangle = \frac{i\,\mathrm{sgn}(s)}{2(n-m)} \min\left\{\frac{\gamma_m(s)}{\gamma_n(s)}, \frac{\gamma_n(s)}{\gamma_m(s)}\right\} \quad \textit{for } m \neq n,$$

where

$$\gamma_n(s) = \left(\frac{\Gamma(n+|s|+1)}{n!}\right)^{1/2}. \tag{26}$$

Proof. Assume that $m < n$ and $s > 0$. Using the explicit expression for the generalized Laguerre polynomials,

$$L_n^{(\alpha)}(x) = \sum_{k=0}^{n}(-1)^k\binom{n+\alpha}{n-k}\frac{1}{k!}\,x^k,$$

one finds that

$$\begin{aligned}\left\langle \varphi_m(s), \dot{H}(s)\varphi_n(s)\right\rangle &= 2s\, c_m(s)\, c_n(s) \\ &\quad \times \int_0^\infty r^{2s-1} L_m^{(s)}\left(\frac{Br^2}{2}\right) L_n^{(s)}\left(\frac{Br^2}{2}\right) \exp\left(-\frac{Br^2}{2}\right) \mathrm{d}r \\ &= s\, c_m(s)\, c_n(s) \left(\frac{2}{B}\right)^s S_{m,n}\end{aligned}$$

where

$$S_{m,n} = \sum_{k=0}^{m}\sum_{\ell=0}^{n}(-1)^{k+\ell}\,\frac{\Gamma(m+s+1)\Gamma(n+s+1)\Gamma(k+\ell+s)}{\Gamma(k+s+1)\Gamma(\ell+s+1)m!n!}\binom{m}{k}\binom{n}{\ell}.$$

In this expression only the summand with $k = 0$ does not vanish since

$$\sum_{\ell=0}^{n}(-1)^\ell\binom{n}{\ell}\ell^j = 0 \quad \text{for } j = 0, 1, \ldots, n-1,$$

Hence

$$\begin{aligned}S_{m,n} &= \frac{\Gamma(m+s+1)\Gamma(n+s+1)}{\Gamma(s+1)m!n!}\sum_{\ell=0}^{n}(-1)^\ell\,\frac{\Gamma(\ell+s)}{\Gamma(\ell+s+1)}\binom{n}{\ell} \\ &= \frac{\Gamma(m+s+1)\Gamma(n+s+1)}{\Gamma(s+1)m!n!}\,B(s, n+1) \\ &= \frac{\Gamma(m+s+1)}{s\,m!}\,.\end{aligned}$$

Furthermore, $\lambda_n(s) - \lambda_m(s) = 2B(n-m)$ and so

$$\langle\varphi_m(0), Q(s)\varphi_n(0)\rangle = i\left(\frac{2}{B}\right)^s \frac{c_m(s)c_n(s)}{2B(n-m)}\,\frac{\Gamma(m+s+1)}{m!}\,.$$

Now it suffices to plug in the explicit expressions for the normalization constants $c_m(s)$ and $c_n(s)$. $\square$

Using the Stirling formula one can check the asymptotic behavior of the matrix entries of the operator $Q(s)$ for m and n large. It turns out that the operator $Q(s)$ is in some sense close to a Hermitian operator $A(s)$ in $L^2(\mathbb{R}_+, r\mathrm{d}r)$ with the matrix entries

$$\langle\varphi_m(0), A(s)\varphi_n(0)\rangle = 0 \quad \text{for } m = n, \tag{27}$$

and

$$\langle\varphi_m(0), A(s)\varphi_n(0)\rangle = \frac{i\,\mathrm{sgn}(s)}{2(n-m)}\,\min\left\{\left(\frac{m+1}{n+1}\right)^{|s|/2}, \left(\frac{n+1}{m+1}\right)^{|s|/2}\right\}$$
$$\text{for } m\neq n. \qquad (28)$$

Note that $A(0+) = Q(0+)$. We shall also write $Q(s)_{mn}$ instead of $\langle\varphi_m(0), Q(s)\varphi_n(0)\rangle$, and similarly for $A(s)$.

Lemma 5. *Let $A(s)$ be the Hermitian operator in $L^2(\mathbb{R}_+, r\,dr)$ defined by relations (27) and (28). Then $Q(s)-A(s)$ is a Hilbert-Schmidt operator and it holds true that*

$$\|Q(s)-A(s)\|_{\mathrm{HS}} \le \frac{1}{2}\,|s|(1+|s|)^{(3+|s|)/2}.$$

Proof. Let us suppose for definiteness that $s>0$ and $m<n$. For $x\ge 1$ set

$$g_s(x) = \frac{\Gamma(x+s)}{x^s\Gamma(x)}\,.$$

One can express

$$\begin{aligned}|Q(s)_{mn}-A(s)_{mn}| &= \frac{1}{2(n-m)}\left|g_s(m+1)^{1/2}-g_s(n+1)^{1/2}\right| \\ &\quad\times\left(\frac{m+1}{n+1}\right)^{s/2} g_s(n+1)^{-1/2} \\ &\le \frac{1}{4}\,g_s(n+1)^{-1/2}\int_0^1 g_s(m+1+(n-m)t)^{-1/2} \\ &\quad\times|g_s'(m+1+(n-m)t)|\,\mathrm{d}t.\end{aligned}$$

Notice that
$$\frac{g_s'(x)}{g_s(x)} = \frac{\Gamma'(x+s)}{\Gamma(x+s)} - \frac{\Gamma'(x)}{\Gamma(x)} - \frac{s}{x}\,.$$

Using the well known formula for the logarithmic derivative of the gamma function,
$$-\frac{\Gamma'(z)}{\Gamma(z)} = \frac{1}{z}+\gamma+\sum_{n=1}^{\infty}\left(\frac{1}{n+z}-\frac{1}{n}\right), \qquad (29)$$

one finds that

$$
\begin{aligned}
\frac{g_s'(x)}{g_s(x)} &= s\left(\sum_{n=0}^{\infty}\frac{1}{(n+x)(n+x+s)}-\frac{1}{x}\right)\\
&\le s\left(\sum_{n=0}^{\infty}\frac{1}{(n+x)^2}-\frac{1}{x}\right)\\
&\le s\left(\frac{1}{x^2}+\int_x^\infty\frac{\mathrm{d}y}{y^2}-\frac{1}{x}\right)\\
&= \frac{s}{x^2}\,.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\frac{g_s'(x)}{g_s(x)} &\ge s\left(\int_x^\infty\frac{\mathrm{d}y}{y(y+s)}-\frac{1}{x}\right)\\
&= \ln\Big(1+\frac{s}{x}\Big)-\frac{s}{x}\\
&\ge -\frac{s^2}{2x^2}\,.
\end{aligned}
$$

In particular,

$$
|g_s'(x)|\le\frac{s(s+1)}{x^2}\,g_s(x).
$$

From here one derives the estimates, for $t\in[0,1]$,

$$
\begin{aligned}
\frac{g_s(m+1+(n-m)t)}{g_s(n+1)} &= \exp\left(-\int_{m+1+(n-m)t}^{n+1}\frac{g_s'(y)}{g_s(y)}\,\mathrm{d}y\right)\\
&\le \exp\left(\int_{m+1}^{n+1}\left(\frac{s}{y}-\ln\Big(\frac{y+s}{y}\Big)\right)\mathrm{d}y\right)\\
&= \exp\bigg((m+1+s)\ln\Big(1+\frac{s}{m+1}\Big)\\
&\qquad -(n+1+s)\ln\Big(1+\frac{s}{n+1}\Big)\bigg)\\
&\le (1+s)^{1+s}
\end{aligned}
$$

and

$$
\begin{aligned}
|Q(s)_{mn}-A(s)_{mn}| &\le \frac{s(s+1)}{4\,g_s(n+1)^{1/2}}\int_0^1\frac{g_s(m+1+(n-m)t)^{1/2}}{(m+1+(n-m)t)^2}\,\mathrm{d}t\\
&\le \frac{1}{4}\,s(1+s)^{(3+s)/2}\int_0^1\frac{\mathrm{d}t}{(m+1+(n-m)t)^2}\,.
\end{aligned}
$$

Let $F(t)$ be a Hermitian operator in $L^2(\mathbb{R}_+, r\mathrm{d}r)$ with the following matrix entries in the basis $\{\varphi_n(0)\}$:

$$F(t)_{mn} = 0 \quad \text{for } m = n,$$

and

$$F(t)_{mn} = (m + 1 + (n - m)t)^{-2} \quad \text{for } m < n.$$

Then $F(t)$ is a Hilbert-Schmidt operator and

$$\begin{aligned} \|F(t)\|_{\mathrm{HS}}^2 &= 2 \sum_{m=0}^{\infty} \sum_{n=m+1}^{\infty} (m + 1 + (n - m)t)^{-4} \\ &\leq 2 \sum_{m=0}^{\infty} \int_0^{\infty} \frac{\mathrm{d}y}{(m + 1 + ty)^4} \\ &= \frac{2}{3t} \sum_{m=0}^{\infty} \frac{1}{(m+1)^3} \\ &\leq \frac{1}{t}\,. \end{aligned}$$

Hence

$$\begin{aligned} \|Q(s) - A(s)\|_{\mathrm{HS}} &\leq \frac{1}{4}\, s(1+s)^{(3+s)/2} \int_0^1 \|F(t)\|_{\mathrm{HS}}\, \mathrm{d}t \\ &\leq \frac{1}{2}\, s(1+s)^{(3+s)/2}. \end{aligned}$$

This proves the lemma. □

Combining Lemma 3 and Lemma 5 we deduce that the operator $Q(s)$ is actually bounded.

Lemma 6. *The operator $Q(s)$ is bounded and its norm satisfies the estimate*

$$\|Q(s)\| \leq \frac{\pi}{2} + 12\,|s| + \frac{1}{2}\,|s|(1 + |s|)^{(3+|s|)/2}.$$

Proof. Let $A(s)$ be the Hermitian operator in $L^2(\mathbb{R}_+, r\mathrm{d}r)$ defined by relations (27) and (28). According to Lemma 3 it holds true that

$$\|A(s)\| \leq \frac{1}{2} \left(\pi + \left(\frac{\sqrt{2}}{3} + 4 \right) \pi^2 \frac{|s|}{2} \right).$$

Lemma 5 leads to the estimate

$$\begin{aligned}
\|Q(s)\| &\leq \|A(s)\| + \|Q(s) - A(s)\| \\
&\leq \frac{1}{2}\left(\pi + \left(\frac{1}{3\sqrt{2}} + 2\right)\pi^2|s| + |s|(1+|s|)^{(3+|s|)/2}\right).
\end{aligned}$$

Since $\big(1 + 1/(6\sqrt{2})\big)\pi^2 < 12$ the lemma follows. □

4 The meaning of the propagator $U_\tau(s, s_0)$

As already discussed in the Introduction the natural propagator $U_\tau(s, s_0)$ defined in (5) is not related in the standard way to the Hamiltonian $\tau H(s)$ defined in (1). In particular it is not clear if $U_\tau(s, s_0)$ maps the domain $\operatorname{Dom} H(s_0)$ into $\operatorname{Dom} H(s)$. This is why we propose in the Appendix the notion of a propagator weakly associated to a Hamiltonian, see Definition A.3. We should like to emphasize that this relationship is unique, i.e. at most one propagator can be weakly associated to a Hamiltonian.

In this section we show that U_τ is weakly associated to τH and that $(s, r) \mapsto U_\tau(s, s_0)\psi_0(r)$ satisfies the Schrödinger equation as a distribution for all $\psi_0 \in L^2(\mathbb{R}_+, r dr d\varphi)$.

Proposition 7. *The propagator $U_\tau(s, s_0)$ is weakly associated to $\tau H(s)$.*

Proof. Relation (5) means that

$$U_\tau(s, s_0) = V(s)e^{-i\tau\Omega(s)}C(s, s_0)e^{i\tau\Omega(s_0)}V(s_0)^{-1}.$$

So starting from $C(s, s_0)$ one can reach $U_\tau(s, s_0)$ by two consecutive unitary transformations. The propagator $C(s, s_0)$ was defined in (6). It corresponds to the Hamiltonian $-Q_\tau(s)$ defined in (7). According to Lemma 6 the function $\|Q_\tau(s)\| = \|Q(s)\|$ is locally bounded and thus $C(s, s_0)$ is given by the Dyson formula, see relation (31) in Section 5.

First we apply Proposition A.4 in which we set $A(t) = -Q_\tau(t)$, $D = \operatorname{Dom} H(0)$, $T(t) = \exp(-i\tau\Omega(t))$ and

$$X(t) = i\left(\partial_t e^{-i\tau\Omega(t)}\right)e^{i\tau\Omega(t)} = \tau W(t).$$

We conclude that the propagator $e^{-i\tau\Omega(s)}C(s, s_0)e^{i\tau\Omega(s_0)}$ is weakly associated to

$$\tau W(s) - e^{-i\tau\Omega(s)}Q_\tau(s)e^{i\tau\Omega(s)} = \tau W(s) - Q(s).$$

Next we apply Proposition A.6 in which we set $\tilde{H}(t) = \tau W(t) - Q(t)$ and $\tilde{U}(t,s) = e^{-i\tau\Omega(t)}C(t,s)e^{i\tau\Omega(s)}$. Recall further that $V(t)$ was defined in (8). We conclude that $U_\tau(s,s_0) = V(s)\tilde{U}(s,s_0)V(s_0)^{-1}$ is weakly associated to

$$\tau V(s)W(s)V(s)^{-1} - V(s)Q(s)V(s)^{-1} + i\dot{V}(s)V(s)^{-1} = \tau H(s).$$

The proposition is proven. $\square$

In the studied model $\mathcal{H} = L^2(\mathbb{R}_+, r\mathrm{d}r)$ and so

$$\mathcal{K} = L^2(\mathbb{R}, \mathcal{H}, \mathrm{d}s) = L^2(\mathbb{R} \times \mathbb{R}_+, r\mathrm{d}s\mathrm{d}r).$$

Let $\mathfrak{H} = \int_{\mathbb{R}}^{\oplus} H(s)\,\mathrm{d}s$ be the direct integral of the family of self-adjoint operators $H(s)$ which is nothing but a multiplication operator in $\mathcal{K}$. Let K_τ be the quasi-energy operator associated to the propagator $U_\tau(s,s_0)$ (see Appendix). According to Proposition 7 it holds true that

$$K_\tau = \overline{-i\partial_s + \tau\mathfrak{H}}\,. \tag{30}$$

To an initial condition $\psi_0 \in \mathcal{H}$ we relate the function $\psi(s,r) = \big(U_\tau(s,0)\psi_0\big)(r)$ which is a locally square integrable function in the variables s and r. We now show that $\psi(s,r)$ fulfills the Schrödinger equation in the space of distributions $\mathscr{D}'(\mathbb{R}\times\,]0,\infty[)$. Let us note that for the proof it suffices to know that $-i\partial_s + \tau\mathfrak{H} \subset K_\tau$, the stronger property (30) is not necessary.

Proposition 8. *For every $\psi_0 \in \mathcal{H}$, the function $\psi(s,r) = \big(U_\tau(s,0)\psi_0\big)(r)$ satisfies the Schrödinger equation in the sense of distributions.*

Proof. Let $\xi \in C_0^\infty(\mathbb{R}\times\,]0,+\infty[)$ be an arbitrary real-valued test function. Set $g(s,r) = \xi(s,r)/r$. Clearly, $g \in \mathrm{Dom}(-i\partial_s + \tau\mathfrak{H}) \subset \mathrm{Dom}\,K_\tau$. Let $[a,b]\times[c,d]$ be a rectangle containing $\mathrm{supp}\,\xi$ and choose $\eta \in C_0^\infty(\mathbb{R})$ so that $\eta \equiv 1$ on a neighborhood of the interval $[a,b]$. From Proposition A.2 we know that $K_\tau(\eta(s)\psi(s,r)) = -i\eta'(s)\psi(s,r)$. From the choice of η it follows that

$$0 = -i\langle g, \eta'\psi\rangle_{\mathcal{K}} = \langle g, K_\tau(\eta\psi)\rangle_{\mathcal{K}} = \langle(-i\partial_s + \tau\mathfrak{H})g, \eta\psi\rangle_{\mathcal{K}}.$$

The last term equals

$$\begin{aligned}
&\int_{\mathbb{R}\times\mathbb{R}_+}\left(i\partial_s\frac{1}{r}\,\xi(s,r) + \tau H(s)\frac{1}{r}\,\xi(s,r)\right)\eta(s)\psi(s,r)\,r\mathrm{d}s\mathrm{d}r\\
&= \int_{\mathbb{R}\times\mathbb{R}_+}\left(i\partial_s\xi(s,r) + \tau\left(-\partial_r r\partial_r\frac{1}{r} + \frac{1}{r^2}\left(s + \frac{Br^2}{2}\right)^2\right)\xi(s,r)\right)\psi(s,r)\,\mathrm{d}s\mathrm{d}r.
\end{aligned}$$

This means that

$$-i\partial_s\psi(s,r) + \tau\left(-\frac{1}{r}\,\partial_r r\partial_r + \frac{1}{r^2}\left(s + \frac{Br^2}{2}\right)^2\right)\psi(s,r) = 0$$

in the domain $\mathbb{R}\times\,]0,+\infty[$ in the sense of distributions. $\square$

5 Proof of the adiabatic theorem

We follow the strategy explained in the Introduction. The adiabatic propagator U_{AD} (see (4)) and the propagator U_τ defined in (5) differ by C defined by (6). Since $Q_\tau(s) = e^{i\tau\Omega(s)}Q(s)e^{-i\tau\Omega(s)}$, defined in (7), is unitarily equivalent to $Q(s)$ it is bounded, uniformly in s on every bounded interval $[0,S]$. Hence $C(s,s_0)$ exists and is given by the Dyson formula:

$$C(s,s_0) = \mathbb{I} + \sum_{n=1}^{\infty} i^n \int_{s_0}^{s} \mathrm{d}s_1 \int_{s_0}^{s_1} \mathrm{d}s_2 \ldots \int_{s_0}^{s_{n-1}} \mathrm{d}s_n\, Q_\tau(s_1)Q_\tau(s_2)\ldots Q_\tau(s_n). \tag{31}$$

The task is to estimate the norm of the integral of Q_τ. This will be done by the integration by parts technique developed in the following two lemmas.

The first step is to find a bounded differentiable solution $X(s)$ of the commutation equation

$$Q(s) = i\,[W(s), X(s)].$$

The operator $W(s)$ was defined in (9). The off-diagonal entries of the $X(s)$ are determined unambiguously,

$$\begin{aligned} \langle\varphi_m(0), X(s)\varphi_n(0)\rangle &= -i\,\frac{\langle\varphi_m(0), Q(s)\varphi_n(0)\rangle}{\lambda_m(s)-\lambda_n(s)} \qquad (32)\\ &= -\frac{\operatorname{sgn}(s)}{4B(n-m)^2}\,\min\left\{\frac{\gamma_m(s)}{\gamma_n(s)}, \frac{\gamma_n(s)}{\gamma_m(s)}\right\} \quad \text{for } m\neq n, \end{aligned}$$

with $\gamma_n(s)$ defined in (26). We set

$$\langle\varphi_m(0), X(s)\varphi_n(0)\rangle = 0 \quad \text{for } m = n, \tag{33}$$

and write again $X(s)_{mn}$ instead of $\langle\varphi_m(0), X(s)\varphi_n(0)\rangle$.

Lemma 9. *The operator $X(s)$ defined by relations (33) and (32) is bounded and its norm satisfies the estimate*

$$\|X(s)\| \leq \frac{\pi^2}{12\,B}\,.$$

The derivative $\dot{X}(s)$ exists in the operator norm and satisfies the estimate

$$\|\dot{X}(s)\| \leq \frac{(1+\sqrt{2})\pi^2}{48\,B}\,.$$

Proof. The operator norm of $X(s)$ is bounded from above by the Shur-Holmgren norm,

$$\|X(s)\| \leq \|X(s)\|_{\mathrm{SH}} = \sup_{m\in\mathbb{Z}_+} \sum_{n=0}^{\infty} |X(s)_{mn}| \leq \frac{1}{2B} \sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{12\,B}\,.$$

Suppose that $s>0$ and $m<n$. Let us estimate the derivative of $X(s)_{mn}$. Using (29) one finds that

$$\begin{aligned}\left(\frac{\gamma_m(s)}{\gamma_n(s)}\right)' &= \frac{\gamma_m(s)}{2\gamma_n(s)} \left(\frac{\Gamma'(m+s+1)}{\Gamma(m+s+1)} - \frac{\Gamma'(n+s+1)}{\Gamma(n+s+1)}\right)\\ &= \frac{\gamma_m(s)}{2\gamma_n(s)} \sum_{k=0}^{\infty} \frac{n-m}{(k+m+s+1)(k+n+s+1)}\,.\end{aligned}$$

Hence

$$\begin{aligned}\left|\frac{\mathrm{d}}{\mathrm{d}s} X(s)_{mn}\right| &\leq \frac{1}{8B(n-m)} \left(\frac{1}{(m+1)(n+1)} + \int_1^{\infty} \frac{\mathrm{d}y}{(y+m)(y+n)}\right)\\ &= \frac{1}{8B(n-m)} \left(\frac{1}{(m+1)(n+1)} + \frac{1}{n-m}\,\ln\!\left(\frac{n+1}{m+1}\right)\right).\end{aligned}$$

Thus we get, for $m \neq n$,

$$\left|\frac{\mathrm{d}}{\mathrm{d}s} X(s)_{mn}\right| \leq \frac{1}{8B} \left(\frac{1}{(m+1)(n+1)} + \frac{1}{|n-m|\min\{m+1,n+1\}}\right). \tag{34}$$

Let $\dot{X}(s)$ be a Hermitian operator in $L^2(\mathbb{R}_+, r\mathrm{d}r)$ with the matrix entries $\mathrm{d}X(s)_{mn}/\mathrm{d}s$. From the estimate (34) we deduce that $\dot{X}(s)$ is a Hilbert-Schmidt operator and

$$\begin{aligned}\|\dot{X}(s)\|_{\mathrm{HS}} &\leq \frac{1}{8B} \left(\sum_{m=0}^{\infty} \frac{1}{(m+1)^2} \sum_{n=0}^{\infty} \frac{1}{(n+1)^2}\right)^{1/2}\\ &\quad + \frac{1}{8B} \left(2 \sum_{m=0}^{\infty} \frac{1}{(m+1)^2} \sum_{n=m+1}^{\infty} \frac{1}{(n-m)^2}\right)^{1/2}\\ &= \frac{(1+\sqrt{2})\pi^2}{48\,B}\,.\end{aligned}$$

Furthermore, since estimate (34) is uniform in s one can apply the Lebesgue dominated convergence theorem to conclude that

$$\lim_{\varepsilon\to 0}\left\|\frac{1}{\varepsilon}\left(X(s+\varepsilon)-X(s)\right)-\dot{X}(s)\right\|_{\mathrm{HS}}=0.$$

Hence the derivative of the operator-valued function $X(s)$ exists in the operator norm and equals $\dot{X}(s)$. □

The matrix entries of the operator $Q_\tau(s)$ defined in (7) equal

$$\langle\varphi_m(0),Q_\tau(s)\varphi_n(0)\rangle = i\,e^{i\tau(\omega_m(s)-\omega_n(s))}\,\langle\varphi_m(s),\dot{\varphi}_n(s)\rangle\,.$$

Notice that the both operators $\Omega(s)$ and $W(s)=\Omega'(s)$ are diagonal in the basis $\{\varphi_n(0)\}$ and therefore they commute.

Lemma 10. *It holds true that*

$$\left\|\int_0^s Q_\tau(u)\,du\right\| \le \left(1+\frac{1+\sqrt{2}}{8}\,|s|\right)\frac{\pi^2}{6B\tau}\,.$$

Proof. Suppose that $s>0$. The integral can be rewritten as follows,

$$\begin{aligned}\int_0^s Q_\tau(u)\,\mathrm{d}u \;&=\; i\int_0^s e^{i\tau\Omega(u)}[W(u),X(u)]\,e^{-i\tau\Omega(u)}\,\mathrm{d}u\\ &= \frac{1}{\tau}\int_0^s\left(\left(e^{i\tau\Omega(u)}\right)'X(u)\,e^{-i\tau\Omega(u)}+e^{i\tau\Omega(u)}X(u)\left(e^{-i\tau\Omega(u)}\right)'\right)\mathrm{d}u\\ &= \frac{1}{\tau}\int_0^s\left(\left(e^{i\tau\Omega(u)}X(u)\,e^{-i\tau\Omega(u)}\right)'-e^{i\tau\Omega(u)}\dot{X}(u)e^{-i\tau\Omega(u)}\right)\mathrm{d}u\,.\end{aligned}$$

Consequently,

$$\begin{aligned}\int_0^s Q_\tau(u)\,\mathrm{d}u \;&=\; \frac{1}{\tau}\Bigg(e^{i\tau\Omega(s)}X(s)\,e^{-i\tau\Omega(s)}-X(0)\\ &\qquad -\int_0^s e^{i\tau\Omega(u)}\dot{X}(u)e^{-i\tau\Omega(u)}\,\mathrm{d}u\Bigg).\end{aligned}$$

More precisely, the derivation of this equality was rather formal but it becomes rigorous when sandwiching the both sides with the scalar product $\langle\varphi_m(0),\cdot\,\varphi_n(0)\rangle$. This is to say that the both sides have the same matrix entries in the basis $\{\varphi_n(0)\}$. But since the equality concerns bounded operators it holds true.

Using Lemma 9 one arrives at the estimate

$$
\begin{aligned}
\left\| \int_0^s Q_\tau(u)\,\mathrm{d}u \right\| &\le \frac{1}{\tau}\left(\|X(s)\| + \|X(0)\| + \int_0^s \|\dot{X}(u)\|\,\mathrm{d}u \right) \\
&\le \frac{\pi^2}{B\tau}\left(\frac{1}{6} + \frac{1+\sqrt{2}}{48}\,s \right).
\end{aligned}
$$

The lemma is proven. $\square$

We can now show that the adiabatic propagator $U_{AD}(s,0)$ (see (4)) is close to the propagator $U_\tau(s,0) = U_{AD}(s,0)C(s,0)$ defined in (5) provided the adiabatic parameter τ is large.

Proposition 11. *It holds true that*

$$
\|U_\tau(s,0) - U_{AD}(s,0)\| \le M(s)\, e^{|s|M(s)} \frac{\pi}{3B\tau}
$$

where

$$
M(s) = \frac{\pi}{2} + 12\,|s| + \frac{1}{2}\,|s|(1+|s|)^{(3+|s|)/2}. \tag{35}
$$

Proof. According to Lemma 6, $\|Q(s)\| \le M(s)$, and from Lemma 10 one easily deduces that

$$
\left\| \int_0^s Q_\tau(u)\,\mathrm{d}u \right\| \le \frac{\pi}{3B\tau}\, M(s).
$$

Using formula (5) one can estimate

$$
\begin{aligned}
\|U_\tau(s,0) - U_{AD}(s,0)\| &= \|C(s,0) - \mathbb{I}\| \\
&\le \sum_{n=1}^{\infty} \int_0^{|s|} \mathrm{d}s_1 \ldots \int_0^{s_{n-2}} \mathrm{d}s_{n-1}\, \|Q_\tau(s_1)\| \ldots \|Q_\tau(s_{n-1})\| \\
&\quad \times \left\| \int_0^{s_{n-1}} \mathrm{d}s_n\, Q_\tau(s_n) \right\| \\
&\le \frac{\pi}{3B\tau} \sum_{n=1}^{\infty} M(s)^n \int_0^{|s|} \mathrm{d}s_1 \ldots \int_0^{s_{n-2}} \mathrm{d}s_{n-1} \\
&= \frac{\pi}{3B\tau} \sum_{n=1}^{\infty} M(s)^n \frac{|s|^{n-1}}{(n-1)!}.
\end{aligned}
$$

The proposition is proven. $\square$

6 The general dependence on time

Here we show that the adiabatic theorem extends to Hamiltonians of the form

$$H^\zeta(s) = H\big(\zeta(s)\big)$$

where $H(s)$ is defined in (1) and $\zeta \in C^2(\mathbb{R})$ is a real-valued function. In order to simplify the discussion and to avoid considering discontinuities (recall that $Q(s)$ is discontinuous at $s = 0$) we shall further assume that $\zeta'(s) > 0$ and $\zeta(0) = 0$.

Set

$$V^\zeta(s) = V\big(\zeta(s)\big),\ W^\zeta(s) = W\big(\zeta(s)\big),\ \Omega^\zeta(s) = \int_0^s W^\zeta(u)\,\mathrm{d}u.$$

Let $C^\zeta(s, s_0)$ be the propagator related via the Dyson formula to the Hamiltonian $-Q^\zeta_\tau(s)$ where

$$Q^\zeta_\tau(s) = \exp\big(i\tau\Omega^\zeta(s)\big)\, Q^\zeta(s) \exp\big(-i\tau\Omega^\zeta(s)\big)\,,\ Q^\zeta(s) = \zeta'(s)Q\big(\zeta(s)\big).$$

Exactly in the same way as in the proof of Proposition 7 one can show that the propagator

$$U^\zeta_\tau(s, s_0) = V^\zeta(s) \exp\big(-i\tau\Omega^\zeta(s)\big)\, C^\zeta(s, s_0) \exp\big(i\tau\Omega^\zeta(s_0)\big)\, V^\zeta(s_0)^{-1}$$

is weakly associated to the Hamiltonian $H^\zeta(s)$. The adiabatic propagator now reads

$$U^\zeta_{AD}(s, s_0) = V^\zeta(s) \exp\big(-i\tau\big(\Omega^\zeta(s) - \Omega^\zeta(s_0)\big)\big)\, V^\zeta(s_0)^{-1}.$$

Proposition 12. *Assume that $\zeta \in C^2(\mathbb{R})$, $\zeta'(s) > 0$ and $\zeta(0) = 0$. Then there exists a locally bounded function $m^\zeta(s)$ such that*

$$\forall s \in \mathbb{R},\ \ \Big\|U^\zeta_\tau(s, 0) - U^\zeta_{AD}(s, 0)\Big\| \le \frac{m^\zeta(s)}{B\tau}\,.$$

Proof. Suppose for definiteness that $s > 0$. Recall that $\|Q(s)\| \le M(s)$ where $M(s)$ was defined in (35). The operator-valued function

$$X^\zeta(s) = \zeta'(s)X(\zeta(s)),$$

with $X(s)$ being defined in (32) and (33), satisfies the commutation equation

$$Q^\zeta(s) = i\,[W^\zeta(s), X^\zeta(s)].$$

Quite analogously as in the proof of Lemma 10 one derives the estimate

$$\left\| \int_0^s Q_\tau^\zeta(u)\,\mathrm{d}u \right\| \leq \frac{1}{\tau} \left(\|X^\zeta(s)\| + \|X^\zeta(0)\| + \int_0^s \|\dot{X}^\zeta(u)\|\,\mathrm{d}u \right).$$

In virtue of Lemma 9 we have

$$\|X^\zeta(s)\| \leq \frac{\pi^2}{12B}\,\zeta'(s)$$

and

$$\int_0^s \|\dot{X}^\zeta(u)\|\,\mathrm{d}u \leq \frac{\pi^2}{12B} \int_0^s |\zeta''(u)|\,\mathrm{d}u + \frac{(1+\sqrt{2})\pi^2}{48B} \int_0^s \zeta'(u)^2\,\mathrm{d}u\,.$$

Hence

$$\left\| \int_0^s Q_\tau^\zeta(u)\,\mathrm{d}u \right\| \leq \frac{q^\zeta(s)}{B\tau}$$

where

$$q^\zeta(s) = \frac{\pi^2}{12} \left(\zeta'(0) + \sup_{0\leq u\leq s} \zeta'(u) + \int_0^s |\zeta''(u)|\,\mathrm{d}u + \frac{1+\sqrt{2}}{4} \int_0^s \zeta'(u)^2\,\mathrm{d}u \right).$$

Finally one can proceed similarly as in the proof of Proposition 11 to derive the estimate

$$\left\| U_\tau^\zeta(s,0) - U_{AD}^\zeta(s,0) \right\| = \left\| C^\zeta(s,0) - \mathbb{I} \right\| \leq \exp\!\left(\int_0^{\zeta(s)} M(v)\,\mathrm{d}v \right) \frac{q^\zeta(s)}{B\tau}\,.$$

This completes the proof. □

Appendix. Propagator weakly associated to a Hamiltonian

By a propagator $U(t,s)$ we mean a family of unitary operators in a separable Hilbert space $\mathcal{H}$ depending on $t, s \in \mathbb{R}$ which satisfies the conditions:

(i) $U(t,s)$ is strongly continuous jointly in t, s,

(ii) the Chapman-Kolmogorov equality is satisfied, i.e.

$$\forall t,s,r \in \mathbb{R},\ U(t,r)U(r,s) = U(t,s).$$

Let $H(t)$, $t \in \mathbb{R}$, be a family of self-adjoint operators in $\mathcal{H}$. The domain may depend on t. The standard way how one relates a propagator $U(t,s)$ to $H(t)$ is based on the following two requirements:

(i) $\forall t, s \in \mathbb{R},\ U(t,s)\big(\operatorname{Dom} H(s)\big) = \operatorname{Dom} H(t)$,

(ii) $\forall \psi \in \operatorname{Dom} H(s), \forall t \in \mathbb{R},\ i\partial_t U(t,s)\psi = H(t)U(t,s)\psi$.

Clearly, if a propagator exists then it is unique. In some situations, however, these requirements may turn out to be unnecessarily strong. In particular this is true for the model studied in the current paper. The heart of the problem is illustrated on the following example.

Let $A(t)$ be a family of bounded Hermitian operators in $\mathcal{H}$ which is uniformly bounded. Then the propagator exits and is given by the Dyson formula. Let us call it $C(t,s)$. Let $D \subset \mathcal{H}$ be a dense linear subspace, and let $T(t)$ be a strongly continuous family of unitary operators such that D is invariant with respect to $T(t)$ and for every $\psi \in D$ there exists the derivative $\partial_t T(t)\psi$. Furthermore, suppose that $X(t) = i\dot{T}(t)T(t)^{-1}$, with $\operatorname{Dom} X(t) = D$, is a self-adjoint operator for all t (the dot designates the derivative). A formal computation gives

$$T(t)\Big(-i\partial_t + A(t)\Big)T(t)^{-1} = -i\partial_t + X(t) + T(t)A(t)T(t)^{-1}.$$

If $C(t,s)$ preserved the domain D then the propagator $T(t)C(t,s)T(s)^{-1}$ would solve the Schrödinger equation for $X(t) + T(t)A(t)T(t)^{-1}$ on D. Thus it is natural to associate it to this family of self-adjoint operators. The hypothesis on $C(t,s)$ need not be, however, satisfied since $A(t)$ is an arbitrary family of bounded operators and so $C(t,s)$ will in general not preserve this domain.

In this appendix we propose a way how to associate a propagator to a given time-dependent Hamiltonian in a weak sense. This association is more general than the standard one (which supposes a constant domain and solving the Schrödinger equation in the strong sense) and it is still unique (i.e.: there is at most one propagator weakly associated to a given time dependent Hamiltonian).

Here we develop this approach only to an extent which makes it possible to apply these ideas to the studied model with a time-dependent Aharonov-Bohm flux. In particular, the described example is covered by Proposition A.4 below.

Let $\mathcal{X}$ be a Banach space. We shall say that a vector-valued function $f : \mathbb{R} \to \mathcal{X}$ is absolutely continuous on $\mathbb{R}$ if it is absolutely continuous on every compact interval $I \subset \mathbb{R}$. By the symbol $\widetilde{AC}(\mathbb{R},\mathcal{X})$ (or just $\widetilde{AC}$ if there is no danger of misunderstanding) we shall denote the space of all absolutely continuous vector-valued functions $f(t)$ such that the derivative $f'(t)$ exists almost everywhere on $\mathbb{R}$. In such a case the function $\|f'(t)\|$ is locally integrable and $f(t) = f(0) + \int_0^t f'(s)\,\mathrm{d}s$ [10, Theorem 3.8.6]. If the Banach space $\mathcal{X}$ has the Radon-Nikodym property then the space $\widetilde{AC}(\mathbb{R},\mathcal{X})$ coincides with the space of absolutely continuous vector-valued functions $AC(\mathbb{R},\mathcal{X})$. Let us recall that $\mathcal{X}$ is said to have the Radon-Nikodym property if the fundamental theorem of calculus holds, i.e. if any absolutely continuous function is the antiderivative of a Bochner integrable function. For example, separable Hilbert spaces are known to have the Radon-Nikodym property [6].

Clearly, if $f, g \in AC(\mathbb{R},\mathcal{H})$ then the function $\langle f(t), g(t)\rangle$ is absolutely continuous and

$$\partial_t \langle f(t), g(t)\rangle = \langle f'(t), g(t)\rangle + \langle f(t), g'(t)\rangle \text{ a.e.}$$

Similarly, if $A \in \widetilde{AC}(\mathbb{R},\mathcal{B}(\mathcal{H}))$ and $f \in AC(\mathbb{R},\mathcal{H})$ then $A(t)f(t) \in AC(\mathbb{R},\mathcal{H})$ and

$$\partial_t A(t)f(t) = \dot{A}(t)f(t) + A(t)f'(t) \text{ a.e.}$$

Let $\{e_k\}$ be an orthonormal basis in $\mathcal{H}$. A vector-valued function $f(t) = \sum \eta_k(t)e_k$ belongs to $AC(\mathbb{R},\mathcal{H})$ if and only if the following two conditions are satisfied:

(i) $\exists a \in \mathbb{R}$ such that $\sum_k |\eta_k(a)|^2 < \infty$,

(ii) $\forall k,\ \eta_k \in AC$, and $\left(\sum_k |\eta_k'(t)|^2\right)^{1/2} \in L^1_{\mathrm{loc}}(\mathbb{R})$.

From here one easily derives the following criterion (alternatively, one can again consult [10, Theorem 3.8.6]).

Lemma A.1. *A vector-valued function $f : \mathbb{R} \to \mathcal{H}$ belongs to $AC(\mathbb{R},\mathcal{H})$ if and only if the following two conditions are satisfied:*

(i) there exists a total set $\mathcal{T} \subset \mathcal{H}$ such that for all $\psi \in \mathcal{T}$, $\langle \psi, f(t)\rangle$ is absolutely continuous,

(ii) the derivative $f'(t)$ exists a.e. and $\|f'(t)\| \in L^1_{\mathrm{loc}}(\mathbb{R})$.

Set $\mathcal{K} = L^2(\mathbb{R},\mathcal{H},\mathrm{d}t)$. Let us recall that to every propagator $U(t,s)$ on $\mathcal{H}$ one can relate a unique self–adjoint operator K in $\mathcal{K}$ which is the generator of the one-parameter group of unitary operators $\exp(-i\sigma K)$, $\sigma \in \mathbb{R}$, defined by

$$\left(e^{-i\sigma K} f\right)(t) = U(t, t-\sigma) f(t-\sigma)$$

[11]. K is called the quasi-energy operator. Equivalently,

$$K = \mathfrak{U}(-i\partial_t)\mathfrak{U}^* \quad \text{where } \mathfrak{U} = \int_{\mathbb{R}}^{\oplus} U(t,0)\,\mathrm{d}t. \tag{A.1}$$

So $f \in \operatorname{Dom} K$ if and only if $U(t,0)^{-1}f(t) \in \operatorname{Dom}(-i\partial_t)$ which means that $f \in L^2$, $U(t,0)^{-1}f(t) \in AC$ and $\big(U(t,0)^{-1}f(t)\big)' \in L^2$.

From (A.1) one concludes that the spectrum of K is purely absolutely continuous and coincides with $\mathbb{R}$. So the kernel of K is always trivial. It seems to be natural, however, to introduce a generalized kernel of K, called $\operatorname{Ker}_0 K$, as follows:

$$\begin{aligned}\operatorname{Ker}_0 K \;=\; & \{f \in L^2_{\mathrm{loc}}(\mathbb{R},\mathcal{H},\mathrm{d}t);\ \forall \eta \in C_0^\infty(\mathbb{R}),\ \eta f \in \operatorname{Dom} K \\ & \text{and } K(\eta f) = -i\eta' f\}.\end{aligned}$$

Since K can be very roughly imagined as the formal operator $-i\partial_t + H(t)$ the elements of $\operatorname{Ker}_0 K$ can be regarded as solutions of the Schrödinger equation in a weak sense.

Proposition A.2. *Let $U(t,s)$ be a propagator and let K be the quasi-energy operator associated to it. Then it holds*

$$\operatorname{Ker}_0 K = \{U(t,0)\psi;\ \psi \in \mathcal{H}\}.$$

Proof. If $f(t) = U(t,0)\psi$, with $\psi \in \mathcal{H}$, and $\eta \in C_0^\infty(\mathbb{R})$ then, in $\mathcal{K}$, there exists the derivative

$$i\,\frac{\mathrm{d}}{\mathrm{d}\sigma}\big(e^{-i\sigma K}\eta f\big)(t)\Big|_{\sigma=0} = i\,\frac{\mathrm{d}}{\mathrm{d}\sigma}\big(\eta(t-\sigma)U(t,0)\psi\big)\Big|_{\sigma=0} = -i\eta'(t)f(t).$$

Hence, by the Stone theorem, $\eta f \in \operatorname{Dom} K$ and $K(\eta f) = -i\eta' f$.

Conversely, suppose that $f \in \operatorname{Ker}_0 K$ and set $g(t) = U(t,0)^{-1}f(t)$. Let η be a test function. From (A.1) one deduces that $\eta g \in \operatorname{Dom}(-i\partial_t)$ and

$$\partial_t\big(\eta(t)g(t)\big) = \eta'(t)g(t) \text{ a.e.}$$

Since $\eta \in C_0^\infty(\mathbb{R})$ is arbitrary this implies that $g(t) \in AC(\mathbb{R},\mathcal{H})$ and $g'(t) = 0$ a.e. Consequently, $g(t) = \psi \in \mathcal{H}$ is a constant vector-valued function and $f(t) = U(t,0)\psi$. $\square$

It is known that the correspondence between the propagators and the quasi-energy operators is one-to-one [11, Remark (1) on p.321]. On one hand, by the very definition, K is unambiguously determined by $U(t,s)$. On the other hand, if $U(t,s)$ and $U_1(t,s)$ are two propagators with equal quasi-energy operators, $K = K_1$, then $U(t,s) = U_1(t,s)$. This uniqueness result is also a straightforward corollary of Proposition A.2. Actually, Proposition A.2 implies that for every $\psi \in \mathcal{H}$ there exists $\psi_1 \in \mathcal{H}$ such that $U(t,0)\psi = U_1(t,0)\psi_1$ for all t (we use the strong continuity of the propagators). By setting $t = 0$ one finds that $\psi = \psi_1$. Hence $U(t,0)\psi = U_1(t,0)\psi$ for all $\psi \in \mathcal{H}$. Consequently,

$$U(t,s) = U(t,0)U(s,0)^{-1} = U_1(t,0)U_1(s,0)^{-1} = U_1(t,s).$$

For a family of self-adjoint operators $H(t)$, $t \in \mathbb{R}$, set $\mathfrak{H} = \int_{\mathbb{R}}^{\oplus} H(t)\,\mathrm{d}t$. This means that $f \in \mathcal{K}$ belongs to $\operatorname{Dom}\mathfrak{H}$ if and only if $f(t) \in \operatorname{Dom} H(t)$ a.e. and $\|H(t)f(t)\| \in L^2(\mathbb{R}, \mathrm{d}t)$. Then $\mathfrak{H}$ is a self-adjoint operator in $\mathcal{K}$. In what follows we shall always suppose that the intersection $\operatorname{Dom}(-i\partial_t) \cap \operatorname{Dom}\mathfrak{H}$ is dense in $\mathcal{K}$. For example, this is true in the case when the domain $\operatorname{Dom} H(t)$ is independent of t. Consequently, $-i\partial_t + \mathfrak{H}$ is a densely defined symmetric operator.

Definition A.3. *We shall say that a propagator $U(t,s)$ is* weakly associated *to $H(t)$ if*

$$K = \overline{-i\partial_t + \mathfrak{H}}\,. \tag{A.2}$$

Notice that equality (A.2) is equivalent to the following two conditions:

(i) $-i\partial_t + \mathfrak{H} \subset K$,

(ii) $-i\partial_t + \mathfrak{H}$ is essentially self-adjoint.

Furthermore, it is important to note that this definition still guarantees the uniqueness, i.e. to $H(t)$ one can weakly associate at most one propagator $U(t,s)$. Actually, if $U(t,s)$ and $U_1(t,s)$ are weakly associated to $H(t)$ then $K = K_1$ according to equality (A.2). But due to the one-to-one correspondence between the propagators and the quasi-energy operators we have $U(t,s) = U_1(t,s)$.

Now we are ready to formulate and prove two propositions which are directly applicable to the model studied in this paper.

Proposition A.4. *Let $A(t)$ be a family of bounded self–adjoint operators in $\mathcal{H}$ which is locally bounded. Let $C(t,s)$ be the propagator associated to $A(t)$ via the Dyson formula. Let $D \subset \mathcal{H}$ be a dense linear subspace and let $T(t)$ be a strongly continuous family of unitary operators in $\mathcal{H}$ obeying the conditions:*

(i) $\forall t \in \mathbb{R},\ T(t)D = D$,

(ii) $\forall \psi \in D$*, $T(t)\psi$ is continuously differentiable,*

(iii) $\forall t \in \mathbb{R}$*, $X(t) = i\dot{T}(t)T(t)^{-1}$, with* $\operatorname{Dom} X(t) = D$*, is a self-adjoint operator.*

Then the propagator $T(t)C(t,s)T(s)^{-1}$ is weakly associated to the family $X(t) + T(t)A(t)T(t)^{-1}$.

Proof. Set

$$Y(t) = X(t) + T(t)A(t)T(t)^{-1},\ \mathfrak{Y} = \int_{\mathbb{R}}^{\oplus} Y(t)\,\mathrm{d}t,\ \mathfrak{T} = \int_{\mathbb{R}}^{\oplus} T(t)\,\mathrm{d}t.$$

Let K_Y be the quasi-energy operator associated to the propagator $T(t)C(t,s)T(s)^{-1}$. Set

$$C(t) = C(t,0),\ \mathfrak{C} = \int_{\mathbb{R}}^{\oplus} C(t)\,\mathrm{d}t.$$

$C(t)$ is a family of unitary operators which satisfies $C(t) \in \widetilde{AC}(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ and $A(t) = i\dot{C}(t)C(t)^{-1}$.

(i) Let us verify that

$$-i\partial_t + \mathfrak{Y} \subset K_Y = \mathfrak{T}\mathfrak{C}(-i\partial_t)\mathfrak{C}^{-1}\mathfrak{T}^{-1}.$$

Suppose that a vector-valued function $f : \mathbb{R} \to \mathcal{H}$ belongs to $\operatorname{Dom}(-i\partial_t + \mathfrak{Y})$. This happens if and only if f obeys the conditions: $f \in L^2$, $f \in AC$, $f' \in L^2$, $f(t) \in D$ a.e. and $Y(t)f(t) \in L^2$. In that case the function $T(t)^{-1}f(t)$ is differentiable a.e. and the derivative

$$\big(T(t)^{-1}f(t)\big)' = T(t)^{-1}\big(f'(t) + iX(t)f(t)\big)$$

is square integrable. Moreover, if $\psi \in D$ then the function $\langle \psi, T(t)^{-1}f(t)\rangle = \langle T(t)\psi, f(t)\rangle$ is absolutely continuous. According to Lemma A.1 this implies that $T(t)^{-1}f(t) \in AC(\mathbb{R}, \mathcal{H})$ and consequently $C(t)^{-1}T(t)^{-1}f(t) \in AC$ as well. Furthermore, a straightforward computation yields

$$\begin{aligned} Y(t)f(t) &= i\left(\dot{T}(t)T(t)^{-1}f(t) + T(t)\dot{C}(t)C(t)^{-1}T(t)^{-1}f(t)\right) \\ &= i\big(T(t)C(t)\big)'C(t)^{-1}T(t)^{-1}f(t) \\ &= if'(t) - iT(t)C(t)\left(C(t)^{-1}T(t)^{-1}f(t)\right)'. \end{aligned}$$

Hence $(C(t)^{-1}T(t)^{-1}f(t))' \in L^2$, $f \in \operatorname{Dom} K_Y$ and $-if'(t) + Y(t)f(t) = K_Y f(t)$.

(ii) Let us verify that $-i\partial_t + \mathfrak{Y}$ is essentially self-adjoint. Suppose that $g \in \mathrm{Dom}(-i\partial_t + \mathfrak{Y})^*$ satisfies $(-i\partial_t + \mathfrak{Y})^* g = zg$ with $\mathrm{Im}(z) \neq 0$. This means that

$$\forall f \in \mathrm{Dom}(-i\partial_t + \mathfrak{Y}),\ \langle(-i\partial_t + \mathfrak{Y})f, g\rangle_{\mathcal{K}} = z\langle f, g\rangle_{\mathcal{K}}.$$

Choose $f(t) = \eta(t)T(t)\psi$ where $\psi \in D$ and $\eta \in C_0^\infty(\mathbb{R})$ is real-valued. Then $f \in \mathrm{Dom}(-i\partial_t + \mathfrak{Y})$ and an easy computation shows that

$$(-i\partial_t + \mathfrak{Y})f(t) = -i\eta'(t)T(t)\psi + \eta(t)T(t)A(t)\psi.$$

Hence for all $\eta \in C_0^\infty(\mathbb{R})$ we have

$$\int_{\mathbb{R}} (i\eta'(t)\langle T(t)\psi, g(t)\rangle + \eta(t)\langle T(t)A(t)\psi, g(t)\rangle)\,\mathrm{d}t = z\int_{\mathbb{R}} \eta(t)\langle T(t)\psi, g(t)\rangle \mathrm{d}t\,.$$

Setting

$$F(t) = \langle T(t)\psi, g(t)\rangle,\ G(t) = \langle T(t)A(t)\psi, g(t)\rangle,$$

we find that

$$-i\partial_t F(t) + G(t) = zF(t) \tag{A.3}$$

in the sense of distributions. Since both $F(t)$ and $G(t)$ are locally integrable, a standard result from the theory of distributions tells us that $F(t)$ is absolutely continuous and equality (A.3) holds true in the usual sense. Moreover, equality (A.3) implies that

$$\partial_t \left(e^{2\,\mathrm{Im}(z)t}|F(t)|^2\right) = 2\,e^{2\,\mathrm{Im}(z)t}\,\mathrm{Im}\big(\overline{F(t)}G(t)\big).$$

Let us now choose an orthonormal basis $\{\psi_k\}$ whose elements all belong to the domain D. Let us write F_k instead of F and G_k instead of G when replacing ψ by ψ_k. We have derived the equality

$$|F_k(t)|^2 = e^{-2\,\mathrm{Im}(z)(t-a)}|F_k(a)|^2 + 2\int_a^t e^{-2\,\mathrm{Im}(z)(t-s)}\,\mathrm{Im}\big(\overline{F_k(s)}G_k(s)\big)\mathrm{d}s \tag{A.4}$$

which is valid for all k and all $a, t \in \mathbb{R}$. Observe that

$$\sum_k |F_k(t)|^2 = \|g(t)\|^2 \text{ a.e.,}$$
$$\sum_k |F_k(s)||G_k(s)| \leq \|g(s)\|\,\|A(s)T(s)^{-1}g(s)\| \in L^1_{\mathrm{loc}}(\mathbb{R}, \mathrm{d}s) \text{ a.e.,}$$

and

$$\sum_k \overline{F_k(s)}G_k(s) = \big\langle g(s), T(s)A(s)T(s)^{-1}g(s)\big\rangle \in \mathbb{R} \text{ a.e.}$$

Summing in k in equality (A.4) we find that

$$\|g(t)\| = e^{-\operatorname{Im}(z)(t-a)}\|g(a)\|$$

for almost all $a, t \in \mathbb{R}$. Since $\|g(t)\|$ is square integrable this is possible only if $g(t) = 0$ a.e. □

Proposition A.4 has a corollary justifying the adverb "weakly" in Definition A.3.

Corollary A.5. *Assume that a propagator $U(t, t_0)$ is associated as a strong solution of the Schrödinger equation to a time-dependent Hamiltonian $H(t)$ which has, however, a time-independent domain (i.e. the relationship between the propagator and the Hamiltonian is the usual one). Then $U(t, t_0)$ is weakly associated to $H(t)$.*

Proof. In Proposition A.4 it suffices to set $D = \operatorname{Dom} H(0)$, $T(t) = U(t, 0)$ and $A(t) = 0$. Then $X(t) = H(t)$, $C(t, s) = \mathbb{I}$ and $T(t)C(t, s)T(s)^{-1} = U(t, s)$. □

Proposition A.6. *Suppose that $V(t)$, $t \in \mathbb{R}$, is a family of unitary operators which is continuously differentiable in the strong sense. Let $\tilde{H}(t)$, $t \in \mathbb{R}$, be a family of self-adjoint operators such that* $\operatorname{Dom} \tilde{H}(t) = D$ *for all $t \in \mathbb{R}$. Set*

$$H(t) = V(t)\tilde{H}(t)V(t)^{-1} + i\dot{V}(t)V(t)^{-1}.$$

If the propagator $\tilde{U}(t, s)$ is weakly associated to $\tilde{H}(t)$ then the propagator $U(t, s) = V(t)\tilde{U}(t, s)V(s)^{-1}$ is weakly associated to $H(t)$.

Proof. Set

$$\tilde{U}(t) = \tilde{U}(t, 0),\ \tilde{\mathfrak{U}} = \int_{\mathbb{R}}^{\oplus} \tilde{U}(t)\,\mathrm{d}t,\ \mathfrak{V} = \int_{\mathbb{R}}^{\oplus} V(t)\,\mathrm{d}t\,.$$

By the assumption, $\tilde{\mathfrak{U}}(-i\partial_t)\tilde{\mathfrak{U}}^{-1} = \overline{-i\partial_t + \tilde{\mathfrak{H}}}$. We have to show that

$$\mathfrak{V}\tilde{\mathfrak{U}}(-i\partial_t)\tilde{\mathfrak{U}}^{-1}\mathfrak{V}^{-1} = \overline{-i\partial_t + \mathfrak{H}}\,.$$

Since

$$\mathfrak{V}\tilde{\mathfrak{U}}(-i\partial_t)\tilde{\mathfrak{U}}^{-1}\mathfrak{V}^{-1} = \mathfrak{V}\overline{(-i\partial_t + \tilde{\mathfrak{H}})}\mathfrak{V}^{-1} = \overline{\mathfrak{V}(-i\partial_t + \tilde{\mathfrak{H}})\mathfrak{V}^{-1}}$$

it is sufficient to verify that

$$\mathfrak{V}(-i\partial_t + \tilde{\mathfrak{H}})\mathfrak{V}^{-1} = -i\partial_t + \mathfrak{H}.$$

This would also imply that $\mathrm{Dom}(-i\partial_t) \cap \mathrm{Dom}(\mathfrak{H})$ is dense in $\mathcal{K}$.

A vector-valued function $f : \mathbb{R} \to \mathcal{H}$ belongs to $\mathrm{Dom}\big(\mathfrak{V}(-i\partial_t + \tilde{\mathfrak{H}})\mathfrak{V}^{-1}\big)$ if and only if it satisfies the conditions: $f \in L^2$, $V(t)^{-1}f(t) \in AC$, $(V(t)^{-1}f(t))' \in L^2$, $V(t)^{-1}f(t) \in D$ a.e. and $\tilde{H}(t)V(t)^{-1}f(t) \in L^2$. Let us note that from the continuous differentiability of $V(t)$ in the strong sense and from the uniform boundedness principle it follows that $\dot{V}(t)$, $t \in \mathbb{R}$, is a family of bounded operators which is locally bounded. Furthermore, $V(t)^* = V(t)^{-1}$ is continuously differentiable in the strong sense as well and $V(t)^{-1}\psi \in AC$ for all $\psi \in \mathcal{H}$. Suppose that $f \in L^2$. If $V(t)^{-1}f(t) \in AC$ then $f'(t)$ exists a.e. and $\|f'(t)\|$ is locally integrable, the function $\langle \psi, f(t) \rangle = \langle V(t)^{-1}\psi, V(t)^{-1}f(t) \rangle$ is absolutely continuous for all $\psi \in \mathcal{H}$ and therefore, by Lemma A.1, $f(t) \in AC$. Similarly, the converse is also true. If $f(t) \in AC$ then $V(t)^{-1}f(t) \in AC$.

Using these facts and the relation between $\tilde{H}(t)$ and $H(t)$ (including that $\mathrm{Dom}\, H(t) = V(t)D$) one easily finds that the domains of $\mathfrak{V}(-i\partial_t + \tilde{\mathfrak{H}})\mathfrak{V}^{-1}$ and $-i\partial_t + \mathfrak{H}$ coincide and that

$$V(t)\big(-i\partial_t + \tilde{H}(t)\big)V(t)^{-1}f(t) = -if'(t) + H(t)f(t)$$

for every $f \in \mathrm{Dom}(-i\partial_t + \mathfrak{H})$. □

Remark. Proposition A.6 can be easily extended to the case when the family of unitary operators $V(t)$ is continuous and piece-wise continuously differentiable in the strong sense and in each point of discontinuity there exist the limits of the derivative both from the left and from the right.

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