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Franco Fagnola
Politecnico di Milano, Milan, 20133, Italy, franco.fagnola@polimi.it

Zheng Li
Politecnico di Milano, Milan, 20133, Italy, zheng.li@polimi.it

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ON DISTRIBUTIONS OF SELF-ADJOINT EXTENSIONS OF SYMMETRIC OPERATORS

FRANCO FAGNOLA AND ZHENG LI*

Abstract. In quantum probability a self-adjoint operator on a Hilbert space determines a real random variable and one can define a probability distribution with respect to a given state. In this paper we consider self-adjoint extensions of certain symmetric operators, such as momentum and Hamiltonian operators, with various boundary conditions, explicitly compute their probability distributions in some state and study dependence of these probability distributions on boundary conditions.

1. Introduction

In Quantum Probability a self-adjoint operator defines a real random variable. Precisely, any self-adjoint operator A on Hilbert space $\mathcal{H}$ determines a probability measure by $B \mapsto \langle u, P^A(B)u\rangle$, where $u \in \mathcal{H}$ is a unit vector and P^A is the projection-valued measure associated with A. The problem of studying the probability distribution of A with respect to some state $u \in \mathcal{H}$ naturally arises. In particular, the problem of finding the vacuum state distribution of field operators in interacting Fock spaces has recently attracted a lot of interest (see [2, 3, 5] and the references therein).

When the self-adjoint operator is an extension of a symmetric operator, it is interesting to understand the dependence of the distribution on the special self-adjoint extension chosen. This problem is highly non-trivial because different self-adjoint extensions define non-commuting random variables and, moreover, they do not have a common essential domain. In addition, it may not be possible to determine the distribution computing moments, as usually done for field operators in interacting Fock spaces (see [1, 5]), because either moments do not exist or the distribution is not determined by moments.

In this paper, we consider momentum (imaginary unit i times the first derivative) and Hamiltonian (minus second derivative) operators defined on compactly supported smooth functions on $(0, 1)$ or $(0, +\infty)$, and self-adjoint extensions of their closures in $L^2(0, 1)$ or $L^2(0, +\infty)$.

The paper is organized as follows. In Section 2 we compute explicitly the distributions of self-adjoint extensions of momentum on $L^2(0, 1)$ finding a family of discrete distributions (Theorem 2.1) without moments, except in the special

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* Corresponding author.

case where one gets the delta δ_0 at 0 with respect to the pure state determined by the constant function $\mathbb{1}$ equal to 1. This result can be achieved either by a spectral theoretic or a probabilistic method.

In Section 3 we consider self-adjoint extensions of minus second derivative on smooth compactly supported functions on $(0,+\infty)$. These are determined by boundary conditions $u'(0)+ru(0)=0$ ($r\in\mathbb{R}$) or $u(0)=0$. In this case the spectrum is the half-line $[0,+\infty)$ for $r\le 0$ and $\{-r^2\}\cup[0,+\infty)$ for $r>0$ (Proposition 3.1). We can compute explicitly the distribution of self-adjoint extensions with respect to some reference states related with Hermite polynomials in the special cases where the boundary condition is $u'(0)=0$ or $u(0)=0$. Indeed, we find the explicit formula for the Laplace transform of the distribution and, after inversion, we get a family of Gamma distributions (Theorem 3.2). Apparently, this computation does not give an explicit (invertible) Laplace transform for $r\neq 0$.

Finally, in Section 4 we consider self-adjoint extensions of minus second derivative on smooth compactly supported functions on $(0,1)$. In this case boundary conditions become more complicated therefore we consider only some special cases. We compute the Laplace transform of the distribution, which can be easily tackled by separation of variables, and find a collection of discrete distributions (Theorem 4.1) with respect to the reference state $\mathbb{1}$ after the inversion.

Throughout the paper we write $L^2(I)$ for some interval $I\subset\mathbb{R}$ to denote $L^2(I;\mathbb{C})$, i.e. we consider the complex-valued functions.

2. The Momentum Operator on $L^2(0,1)$

The momentum operator on $L^2(0,1)$ can be defined as a self-adjoint extension of the first-order differential operator A on $L^2(0,1)$, i.e.

$$Au=\mathrm{i}u',\quad \mathcal{D}(A)=\left\{\,u\in H^1(0,1)\;\mid\;u(0)=u(1)=0\,\right\}\tag{2.1}$$

Obviously, A is densely-defined, closed and symmetric. As shown in Reed and Simon ([8] Ch.X, Ex.1, p.141), the self-adjoint extensions of A, denoted by A_θ ($0\le\theta<2\pi$), have domain

$$\mathcal{D}(A_\theta)=\left\{u\in H^1(0,1)\;\mid\;u(1)=\mathrm{e}^{-\mathrm{i}\theta}u(0)\right\}.$$

Thus, if we consider as reference state $\mathbb{1}\in L^2(0,1)$, where $\mathbb{1}$ represents the constant function equal to 1, the distribution of A_θ is given by the following

Theorem 2.1. *The self-adjoint extension A_θ of the operator A on $L^2(0,1)$ defined by (2.1), with respect to the state $\mathbb{1}$, has the distribution δ_0 when $\theta=0$ and*

$$\sum_{k\in\mathbb{Z}}\frac{2(1-\cos\theta)}{(\theta+2k\pi)^2}\cdot\delta_{\theta+2k\pi}\tag{2.2}$$

when $0<\theta<2\pi$.

Proof. We first study the point spectrum of the self-adjoint operator A_θ. To this end we solve the eigenvalue problem

$$A_\theta u=\mathrm{i}u'=\lambda u,\quad u\in\mathcal{D}(A_\theta),\quad \lambda\in\mathbb{C},$$

finding solutions

$$u_\lambda(x) = \mathrm{e}^{-\mathrm{i}\lambda x}, \qquad \lambda = \theta + 2k\pi, \quad k \in \mathbb{Z}.$$

Then, we can calculate the probability mass of A_θ at points $\lambda = \theta + 2k\pi$, in the state $\mathbb{1}$. For $\theta \neq 0$ we find

$$\langle \mathbb{1}, A_\theta(\{\lambda\})\,\mathbb{1}\rangle = |\langle u_\lambda, \mathbb{1}\rangle|^2 = \left|\frac{\sin\theta}{\theta + 2k\pi} + \frac{\mathrm{i}(1-\cos\theta)}{\theta + 2k\pi}\right|^2 = \frac{2(1-\cos\theta)}{(\theta + 2k\pi)^2} \tag{2.3}$$

Noting that, for all θ the sequence of functions $(u_{\theta+2k\pi})_{k\in\mathbb{Z}}$ forms a complete orthogonal system in $L^2(0,1)$, and so we found the spectral resolution of A_θ, this proves (2.2). As a byproduct we find the summation formula

$$\sum_{k\in\mathbb{Z}} \frac{2(1-\cos\theta)}{(\theta + 2k\pi)^2} = 1$$

for all $\theta \neq 0$. When $\theta = 0$, we have

$$\langle \mathbb{1}, A_0(\{2k\pi\})\,\mathbb{1}\rangle = \begin{cases} 1, & k = 0 \\ 0, & k \in \mathbb{Z}\setminus\{0\} \end{cases} \tag{2.4}$$

namely, A_0 has the distribution δ_0. $\square$

One may also notice that, if we let $\theta \to 0$ in (2.3), it gives

$$\lim_{\theta\to 0} \frac{2(1-\cos\theta)}{(\theta + 2k\pi)^2} = \begin{cases} 1, & k = 0 \\ 0, & k \in \mathbb{Z}\setminus\{0\} \end{cases}$$

in other words, as a random variable, A_θ converges in distribution to A_0 as $\theta \to 0$.

Remark 2.2. One can get the same conclusion by a probabilistic method first computing explicitly the characteristic function and then the density by Lévy inversion formula. Indeed the unitary group $\left(\mathrm{e}^{\mathrm{i}tA_\theta}\right)_{t\in\mathbb{R}}$ solves the transport equation

$$\frac{\partial u(t,x)}{\partial t} = \mathrm{i}A_\theta u(t,x) = -\frac{\partial u(t,x)}{\partial x}, \quad \forall t \in \mathbb{R}, \quad \forall x \in (0,1)$$

with initial value $u(0,x) = u(x)$ and boundary condition $u(t,1) = \mathrm{e}^{-\mathrm{i}\theta}u(t,0)$. If we assume $\lim_{t\to 0^+} u(t,1) = u(1)$, then the solution will be determined by

$$\begin{cases} u(t,x) = u(x-t) \\ u(t,1) = \mathrm{e}^{-\mathrm{i}\theta}u(t,0) \end{cases} \tag{2.5}$$

Solving the differential equation we find

$$\mathrm{e}^{\mathrm{i}tA_\theta}\mathbb{1}(x) = \mathrm{e}^{([t]+1)\mathrm{i}\theta}1_{[0,t-[t]\,]}(x) + \mathrm{e}^{[t]\mathrm{i}\theta}1_{]t-[t],1]}(x)$$

where $[t]$ denotes the integer part of the real number t and 1_A the indicator function of a Borel set A. Similarly, for $t < 0$,

$$\mathrm{e}^{\mathrm{i}tA_\theta}\mathbb{1}(x) = \mathrm{e}^{[t]\mathrm{i}\theta}1_{[0,t+1-[t]\,]}(x) + \mathrm{e}^{([t]-1)\mathrm{i}\theta}1_{]t+1-[t],1]}(x)$$

Then, the Fourier transform $\phi(t) = \langle \mathbb{1}, \mathrm{e}^{\mathrm{i}tA_\theta}\mathbb{1}\rangle$ of the distribution of A_θ with respect to the state $\mathbb{1}$ becomes

$$\phi(t) = \begin{cases} \mathrm{e}^{([t]+1)\mathrm{i}\theta}(t-[t]) + \mathrm{e}^{[t]\mathrm{i}\theta}(1-(t-[t])), & t>0 \\ \mathrm{e}^{([t]-1)\mathrm{i}\theta}(-(t-[t])) + \mathrm{e}^{[t]\mathrm{i}\theta}(1+(t-[t])), & t<0 \end{cases} \tag{2.6}$$

In order to find the discrete part of the distribution we apply the Lévy inversion formula computing

$$\begin{aligned} \int_{-n}^{n} \mathrm{e}^{-\mathrm{i}ty}\phi(t)dt &= \sum_{k=-n}^{n-1} \int_{k}^{k+1} \mathrm{e}^{-\mathrm{i}ty}\left[\mathrm{e}^{k+1}\theta(t-k) + \mathrm{e}^{\mathrm{i}k\theta}(1-t+k)\right]dt \\ &= \sum_{k=-n}^{n-1}\left[\mathrm{e}^{\mathrm{i}(k+1)(\theta-y)}\frac{1+\mathrm{i}y-\mathrm{e}^{\mathrm{i}y}}{y^2} + \mathrm{e}^{\mathrm{i}k(\theta-y)}\frac{1-\mathrm{i}y-\mathrm{e}^{-\mathrm{i}y}}{y^2}\right] \end{aligned}$$

for $n \geq 1$. Recalling the summation formulae

$$\sum_{k=-n}^{n-1} \mathrm{e}^{\mathrm{i}k(\theta-y)} = \begin{cases} 2n & \text{if } y=\theta+2h\pi \\ \frac{\mathrm{e}^{\mathrm{i}n(\theta-y)}-\mathrm{e}^{-\mathrm{i}n(\theta-y)}}{\mathrm{e}^{\mathrm{i}(\theta-y)}-1} & \text{if } y\neq\theta+2h\pi \end{cases}$$

for $y=\theta$ we find

$$\begin{aligned} \lim_{n\to\infty}\frac{1}{2n}\int_{-n}^{n}\mathrm{e}^{-\mathrm{i}ty}\phi(t)dt &= \lim_{n\to\infty}\frac{1}{2n}\cdot 2n\cdot\left[\frac{1+\mathrm{i}y-\mathrm{e}^{\mathrm{i}y}}{y^2}+\frac{1-\mathrm{i}y-\mathrm{e}^{-\mathrm{i}y}}{y^2}\right] \\ &= \frac{2(1-\cos y)}{y^2} = \frac{2(1-\cos\theta)}{(\theta+2h\pi)^2}\,. \end{aligned}$$

The above limit is 0 for $y\neq\theta$ and we recover the result of Theorem 2.1.

The following corollary summarizes additional properties of distributions of A_θ.

Corollary 2.3. *Let μ_θ be the probability distribution (2.2) on $\mathcal{B}(\mathbb{R})$.*

1. *μ_θ does not have first-order moment,*
2. *If $\theta\neq\theta'$ then μ_θ is not absolutely continuous with respect to $\mu_{\theta'}$,*
3. *The map $\theta\mapsto\mu_\theta$ is continuous with respect to the weak topology on probability measures.*

The proof is immediate.

We disregard the first-order differential operator $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$ on space $L^2(0,+\infty)$ because it does not admit any self-adjoint extension (one can easily check that its deficiency indices are not equal).

3. The Free Particle Hamiltonian on $L^2(0,+\infty)$

In this section we consider the Hamiltonian of a free particle on $(0,+\infty)$, which is the self-adjoint extension of the second-order differential operator A on $L^2(0,+\infty)$ defined as

$$Au=-u'', \quad \mathcal{D}(A)=\{u\in H^2(0,+\infty)\ |\ u(0)=0, u'(0)=0\}$$

It is easy to verify that A is densely-defined, closed and symmetric, and its self-adjoint extensions A_r have domain ([8] Ch.X, Ex.2, p.144)

$$\mathcal{D}(A_r) = \left\{u \in H^2(0,+\infty) \ | \ u'(0) + ru(0) = 0\right\}, \quad r \in \mathbb{R} \tag{3.1}$$

$$\mathcal{D}(A_r) = \left\{u \in H^2(0,+\infty) \ | \ u(0) = 0\right\}, \quad r = \infty \tag{3.2}$$

Before studying the distribution of such A_r, we analyze the spectrum of A_r, which will give us apriori information on the distribution, as we have seen in last section.

3.1. The spectrum of operator A_r. A result by Naimark ([7] Ch.24, Th.5, p.214) describes the spectrum of self-adjoint extensions of symmetric differential operators on $L^2(0,+\infty)$. The continuous spectrum of A_r covers precisely the whole positive half-axis, and the negative half-axis contains at most eigenvalues of finite multiplicity which have no finite point of accumulation on this axis. For our A_r, the discrete part of the spectrum can be described precisely as follows.

Let $z \in \mathbb{C}$, and look for a solution of the eigenvalue problem

$$A_r u = -u'' = zu, \quad u \in \mathcal{D}(A_r) \tag{3.3}$$

Temporarily ignoring the domain of A_r, the equation (3.3) admits solutions

$$u(x) = c_1 \mathrm{e}^{\mathrm{i}\,\zeta x} + c_2 \mathrm{e}^{-\mathrm{i}\,\zeta x} \tag{3.4}$$

where ζ is a square root of z, and c_1, $c_2 \in \mathbb{C}$ are constants. Notice that (3.4) holds when $z \neq 0$. However, when $z = 0$, solutions are linear thus cannot be square integrable on the positive half-axis. Observe that

$$|u(x)|^2 = |c_1|^2 \mathrm{e}^{-2\,\mathrm{Im}\{\zeta\}x} + |c_2|^2 \mathrm{e}^{+2\,\mathrm{Im}\{\zeta\}x} + 2\,\mathrm{Re}\left\{\overline{c_1} c_2 \mathrm{e}^{-2\,\mathrm{Re}\{\zeta\}\mathrm{i}x}\right\}$$

If $\mathrm{Im}\{\zeta\} = 0$, then $u(x) \in L^2(0,+\infty)$ only if $c_1 = c_2 = 0$, and $u(x)$ cannot be an eigenvector. If $\mathrm{Im}\{\zeta\} > 0$, integrability implies $c_2 = 0$, so $u(x) = c_1 \mathrm{e}^{\mathrm{i}\zeta x}$, then

$$\int_0^\infty |u(x)|^2 \mathrm{d}x = |c_1|^2 \int_0^\infty \mathrm{e}^{-2\,\mathrm{Im}\{\zeta\}x} \mathrm{d}x = \frac{|c_1|^2}{2\,\mathrm{Im}\{\zeta\}} < \infty$$

in this case, it is easy to check that $u', u'' \in L^2(0,+\infty)$, then $u \in H^2(0,+\infty)$. The boundary condition $u'(0) + ru(0) = 0$ for $r \in \mathbb{R}$ implies

$$c_1\,(\mathrm{i}\zeta + r) = 0$$

We know $c_1 \neq 0$, otherwise u is not an eigenvector. Thus, we must have $\zeta = \mathrm{i}r$. Then, $r > 0$, and $z = \zeta^2 = -r^2$. On the other hand, if $r = \infty$, then $u(0) = 0$ implies $c_1 = 0$, and u cannot be an eigenvector. If $\mathrm{Im}\{\zeta\} < 0$, we have a similar situation: if we set $c_1 = 0$, then $u(x) = c_2 \mathrm{e}^{-\mathrm{i}\zeta x} \in H^2(0,+\infty)$. Considering the boundary condition, if $r \in \mathbb{R}$, we get $c_2(r - \mathrm{i}\zeta) = 0$, $c_2 \neq 0$ compels $\zeta = -\mathrm{i}r$. Therefore we still have $r > 0$ and $z = \zeta^2 = -r^2$. Also, when $r = \infty$, $u(0) = 0$ implies $c_2 = 0$, then there is no eigenfunction.

As a consequence, only when $0 < r < +\infty$, A_r has a unique eigenvalue $-r^2$, with eigenvectors $u(x) = c\,\mathrm{e}^{-rx}$, $c \in \mathbb{C} \setminus \{0\}$. Otherwise A_r does not have any eigenvalue. After the normalization, we find the eigenvector $u(x) = \sqrt{2r}\,\mathrm{e}^{-rx}$.

We conclude everything in the following proposition:

Proposition 3.1. *Let A_r be the self-adjoint operator defined by (3.1) for $r \in \mathbb{R}$ and (3.2) for $r = \infty$. For all $r \in \mathbb{R} \cup \{\infty\}$, A_r always has the continuous spectrum $[0, +\infty)$; Only when $r > 0$, A_r has the discrete spectrum $\{-r^2\}$ in addition.*

3.2. Distribution of s.a. extensions. Now we go back to the study of the distribution of A_r by Laplace transform. Recall that the semigroup $\left(\mathrm{e}^{-tA_r}\right)_{t\geq 0}$ solves

$$\frac{\partial u(t,x)}{\partial t} = -A_r u(t,x) = \frac{\partial^2 u(t,x)}{\partial x^2}, \quad u(0,x) = u(x) \tag{3.5}$$

which is exactly the heat equation in the one dimensional case with initial datum $u(x)$. Moreover, the boundary conditions are given in (3.1) and (3.2). Borrowing the terminology from the partial differential equations literature, $r = \infty$ corresponds to the Dirichlet problem, $r = 0$ the Neumann problem, $r \in \mathbb{R} \setminus \{0\}$ the Robin problem.

3.2.1. *Dirichlet and Neumman problems.* For $n \geq 0$, we consider the state

$$e_n(x) = \sigma_n (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}x^n} \mathrm{e}^{-\frac{x^2}{2}} = \sigma_n H_n(x) \mathrm{e}^{-\frac{x^2}{2}} \tag{3.6}$$

where $H_n(x)$ denotes the n-th Hermite polynomial, and σ_n the normalization constant.

Theorem 3.2. *For $n \geq 0$ even (resp. odd), the operator A_0 (resp. A_∞) has distribution $\Gamma(n + 1/2, 1)$ with respect to the state e_n.*

Proof. Notice that $e_n(x) \in \mathcal{D}(A_0)$ when n is even, and $e_n(x) \in \mathcal{D}(A_\infty)$ when n is odd, that is to say, the initial values are naturally compatible with the boundary conditions. So the problem can be viewed as global, and the solution of Equation (3.5) is (See [4] Ch.3, Sect.1, p.33), and below $A_n = A_0$ when n is even, $A_n = A_\infty$ when n is odd)

$$\begin{aligned}
\mathrm{e}^{-tA_n} e_n &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{e}^{i\alpha x - \alpha^2 t} \widehat{e}_n(\alpha) \mathrm{d}\alpha \\
&= \frac{\sigma_n}{2\pi} \int_{-\infty}^{+\infty} \mathrm{e}^{i\alpha x} (-1)^n (i\alpha)^n \mathrm{e}^{-\alpha^2 (t+1/2)} \mathrm{d}\alpha \\
&= (-1)^n \frac{\sigma_n}{\sqrt{1+2t}} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \mathrm{e}^{-\frac{x^2}{2(1+2t)}}
\end{aligned}$$

where $\widehat{e}_n$ is the Fourier transform of e_n. Therefore,

$$\left\langle e_n, \mathrm{e}^{-tA_n} e_n \right\rangle = \frac{\sigma_n^2}{\sqrt{1+2t}} \int_0^\infty \frac{\mathrm{d}^n}{\mathrm{d}x^n} \mathrm{e}^{-\frac{x^2}{2}} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \mathrm{e}^{-\frac{x^2}{2(1+2t)}} \mathrm{d}x \tag{3.7}$$

Applying the integration by parts n times for (3.7), one gets

$$\begin{aligned}
\left\langle e_n, \mathrm{e}^{-tA_n} e_n \right\rangle &= \frac{(-1)^n \sigma_n^2}{\sqrt{1+2t}} \int_0^\infty \frac{\mathrm{d}^{2n}}{\mathrm{d}x^{2n}} \mathrm{e}^{-\frac{x^2}{2}} \left(\mathrm{e}^{\frac{x^2}{2}} \mathrm{e}^{-\frac{1+t}{1+2t} x^2} \right) \mathrm{d}x \\
&= \frac{(-1)^n \sigma_n^2}{\sqrt{1+2t}} \cdot \int_0^\infty H_{2n}(x) \cdot \mathrm{e}^{-\frac{1+t}{1+2t} x^2} \mathrm{d}x
\end{aligned} \tag{3.8}$$

Recall that the explicit formula of $H_{2n}(x)$ is

$$H_{2n}(x) = (2n)!\sum_{k=0}^{n}\frac{(-1)^k}{k!(2n-2k)!}\frac{x^{2n-2k}}{2^k} \tag{3.9}$$

Substitution of (3.9) in (3.8) yields,

$$\begin{aligned}
\left\langle e_n, \mathrm{e}^{-tA_n}e_n\right\rangle &= \frac{(-1)^n\sigma_n^2}{\sqrt{1+2t}}(2n)!\sum_{k=0}^{n}\frac{(-1)^k}{k!(2n-2k)!}\frac{1}{2^k}\int_0^\infty x^{2n-2k}\mathrm{e}^{-\frac{1+t}{1+2t}x^2}\mathrm{d}x\\
&= \sqrt{\frac{1+2t}{1+t}}\frac{\sqrt{\pi}(-1)^n\sigma_n^2}{\sqrt{1+2t}}\frac{(2n)!}{2^{n+1}}\sum_{k=0}^{n}\frac{(-1)^k}{k!(2n-2k)!}\frac{(2n-2k-1)!!}{[(1+t)/(1+2t)]^{n-k}}\\
&= \frac{\sqrt{\pi}(-1)^n\sigma_n^2}{\sqrt{1+t}}\frac{(2n)!}{2^{n+1}}\cdot\frac{2^{-n}\left(\frac{1+2t}{1+t}-2\right)^2}{n!}\\
&= \sigma_n^2\cdot\frac{(2n)!}{2^{2n+1}\cdot n!}\sqrt{\pi}\cdot(1+t)^{-n-1/2}
\end{aligned}$$

The remaining problem is to calculate σ_n^2, which is explicitly given by

$$\sigma_n := \left\|(-1)^n\frac{\mathrm{d}^n}{\mathrm{d}x^n}\mathrm{e}^{-\frac{x^2}{2}}\right\|_{L^2(0,\infty)}^{-\frac{1}{2}}$$

In fact,

$$\sigma_n^{-2} = \int_0^\infty\frac{\mathrm{d}^n}{\mathrm{d}x^n}\mathrm{e}^{-\frac{x^2}{2}}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\mathrm{e}^{-\frac{x^2}{2}}\mathrm{d}x = \frac{(2n)!}{2^{2n+1}\cdot n!}\sqrt{\pi} \tag{3.10}$$

It is worth noticing that the integration in (3.10) has the similar form as in (3.7), so the result is immediate. Combining all the parts we obtain the Laplace transform on the distribution

$$\left\langle e_n, \mathrm{e}^{-tA_n}e_n\right\rangle = (1+t)^{-n-1/2} \tag{3.11}$$

The inverse Laplace transform on (3.11) tells us the distribution of A_n with respect to e_n is exactly $\Gamma(n+1/2,1)$. □

3.2.2. *Robin problem.* Following the idea provided by Strauss ([9] Section 3.1, Exercise 5, p.61), we know: when initial value $u(x)$ is regular enough, for solving the Equation 3.5 defined on the positive half-axis with Robin boundary condition, one should extend the initial datum $u(x)$, defined for $x>0$, so that $u'(x)+ru(x)$ is odd on $\mathbb{R}$, and then the Robin solution is determined by

$$u^{(r)}(t,x) = \frac{1}{\sqrt{4\pi t}}\int_{-\infty}^{+\infty}\exp\left\{-\frac{(x-y)^2}{4t}\right\}u(y)\mathrm{d}y \tag{3.12}$$

Therefore, for $x<0$ one should solve the ordinary differential equation

$$u'(x)+ru(x) = -u'(-x)-ru(-x)$$

By the trick multiplying e^{rx} on both sides, we get the extension, as

$$u(x) = u(0)\mathrm{e}^{-rx}+\mathrm{e}^{-rx}\int_x^0\mathrm{e}^{ry}\left[u'(-y)+ru(-y)\right]\mathrm{d}y,\quad x<0 \tag{3.13}$$

For instance, if we choose the unit state $e_r = \sqrt{2r}\mathrm{e}^{-rx}$, $r > 0$, which is exactly the eigenfunction of A_r with corresponding eigenvalue $-r^2$. Then (3.13) implies the extension of $u(x)$ on the negative half-axis is the analytic extension of $u(x)$ defined on positive half-axis. Thus (3.12) gives $\mathrm{e}^{-tA_r}e_r(x) = \sqrt{2r}\exp\{r^2t - rx\}$, and then $\langle e_r(x), \mathrm{e}^{-tA_r}e_r(x)\rangle = \mathrm{e}^{-r^2t}$, which is indeed the Laplace transform of the probability measure δ_{-r^2}, as we expected.

Unfortunately, we have not found a nice state which gives A_r an explicit but non-trivial probability distribution.

4. The Free Particle Hamiltonian on $L^2(0,1)$

Lastly, we consider the free particle Hamiltonian on $L^2(0,1)$ that can be regarded as a self-adjoint extension of the second-order differential operator A defined on $L^2(0,1)$ by

$$Au := -u'', \quad \mathcal{D}(A) = \{u \in H^2(0,1) : u(0) = u(1) = 0,\ u'(0) = u'(1) = 0\}$$

Again, it is easy to check that A is symmetric, closed and densely defined on $L^2(0,1)$. Also, it is well-known the adjoint operator of A, denoted by A^*, is with domain $\mathcal{D}(A^*) = H^2(0,1)$, the whole Sobolev space without any boundary condition.

4.1. Self-adjoint extensions of operator A. We know from the book of Reed and Simon ([8], Th.X.2, p.140) that self-adjoint extensions of A depend on unitary maps on deficiency spaces $\mathcal{K}_+$ to $\mathcal{K}_-$ defined as

$$\mathcal{K}_+ = \mathcal{N}(\mathrm{i} - A^*) = \mathcal{R}(\mathrm{i} + A)^\perp\,,$$
$$\mathcal{K}_- = \mathcal{N}(\mathrm{i} + A^*) = \mathcal{R}(-\mathrm{i} + A)^\perp\,.$$

In this case, solving $(\mathrm{i} - A^*)u = 0$, where $u \in \mathcal{D}(A^*) = H^2(0,1)$, one finds that $\mathcal{N}(\mathrm{i} - A^*)$ is the linear span of the following two base vectors

$$\exp\left\{\frac{-1+\mathrm{i}}{\sqrt{2}}x\right\}, \quad \exp\left\{\frac{1-\mathrm{i}}{\sqrt{2}}x\right\} \tag{4.1}$$

Using the Gram-Schmidt procedure on (4.1), we can get an orthonormal basis in $\mathcal{K}_+$, denoted by ϕ_+ and ϕ_-. The idea can be applied to vectors (4.2) in another deficiency space $\mathcal{K}_-$, namely

$$\exp\left\{\frac{-1-i}{\sqrt{2}}x\right\}, \quad \exp\left\{\frac{1+i}{\sqrt{2}}x\right\} \tag{4.2}$$

After the orthonormalization, one may notice that the obtained orthonormal basis of $\mathcal{K}_-$ consists of $\overline{\phi_+}$ and $\overline{\phi_-}$, i.e. the complex conjugates of ϕ_+ and ϕ_-. Now the unitary maps between deficiency spaces can be characterized by the elements in the unitary group U(2). Then, the domain of self-adjoint extension A_U is

$$\mathcal{D}(A_U) = \{\phi + f + Uf \mid \phi \in \mathcal{D}(A),\ f \in \mathcal{K}_+,\ U \in \mathrm{U}(2)\} \tag{4.3}$$

in which f is a linear combination of the base vectors ϕ_+ and ϕ_-. Now, one sees that finding all the possible self-adjoint extensions and classifying them is not an easy work. Particularly, some derived boundary conditions could be difficult to handle. Since in this paper we focus more on deriving explicit distributions instead of finding and classifying all the self-adjoint extensions, we prefer to choose some typical self-adjoint extensions: at the left boundary, we always have the homogeneous Dirichlet condition $u(0) = 0$, at the right boundary, different kinds of boundary conditions are considered. Mimicking the boundary conditions of last section, at the right boundary, we have the Dirichlet boundary condition when $r = \infty$, Neumann condition when $r = 0$, Robin condition when $r \in \mathbb{R} \setminus \{0\}$. Therefore, we shall define

$$\mathcal{D}(A_r) = \left\{u \in H^2(0,1) \mid u(0) = 0,\ u'(1) + ru(1) = 0\right\}, r \in \mathbb{R} \tag{4.4}$$

$$\mathcal{D}(A_r) = \left\{u \in H^2(0,1) \mid u(0) = 0,\ u(1) = 0\right\}, r = \infty \tag{4.5}$$

Now, we have to prove that they are indeed the self-adjoint extensions of operator A. Additionally, it is easy to verify that A_r is densely-defined, closed and symmetric in any case.

When $r = \infty$. Suppose $\phi \in \mathcal{D}(A_\infty)$ and $\psi \in \mathcal{D}(A_\infty^*)$, then

$$\langle A_\infty \phi, \psi\rangle - \langle \phi, A_\infty^* \psi\rangle = \phi'(0)\overline{\psi}(0) - \phi'(1)\overline{\psi}(1) + \phi(1)\overline{\psi'}(1) - \phi(0)\overline{\psi'}(0) = 0 \tag{4.6}$$

Since we know $\phi(0) = \phi(1) = 0$, then (4.6) implies

$$\phi'(0)\overline{\psi}(0) - \phi'(1)\overline{\psi}(1) = 0$$

holds for arbitrary $\phi \in \mathcal{D}(A_\infty)$. Hence, for ensuring $\psi \in \mathcal{D}(A_\infty^*)$, we must have $\psi(0) = \psi(1) = 0$. Since A_∞ is already symmetric, then it must also be self-adjoint.

When $r \in \mathbb{R}$, by the analogous equality as (4.6), and knowing $\phi'(1) + r\phi(1) = 0$ and $\phi(0) = 0$, the equality

$$\phi(1)\left(\overline{\psi'}(1) - r\overline{\psi}(1)\right) - \phi'(0)\overline{\psi}(0) = 0$$

should hold for all $\phi \in \mathcal{D}(A_r)$. Therefore there must be $\psi'(1) - r\psi(1) = 0$ and $\psi(0) = 0$. So A_r is verified to be self-adjoint.

4.2. Distribution of selected s.a. extensions. We turn to study the distribution of A_r by Laplace transform. We know that $\left(\mathrm{e}^{-tA_r}\right)_{t\geq 0}$ solves

$$\frac{\partial u(t,x)}{\partial t} = -A_r u(t,x) = \frac{\partial^2 u(t,x)}{\partial x^2}, \quad u(0,x) = u(x) \tag{4.7}$$

and the boundary conditions are given in (4.4) and (4.5), respectively.

We consider as reference state $\mathbb{1} \in L^2(0,1)$. The main result of this section can be summarized as the follows:

Theorem 4.1. *The free particle Hamiltonian A_r on $L^2(0,1)$, defined by (4.4), and (4.5) and with respect to state $\mathbb{1}$, always has purely discrete distribution with support contained in $[0,\infty)$. In particular, when $r = \infty$, A_r has the distribution*

$$\sum_{n=0}^{\infty} \frac{8}{(2n+1)^2\pi^2} \cdot \delta_{(2n+1)^2\pi^2} \tag{4.8}$$

When $r = 0$, A_r has the distribution

$$\sum_{n=0}^{\infty} \frac{2}{(n+1/2)^2\pi^2} \cdot \delta_{(n+1/2)^2\pi^2} \tag{4.9}$$

When $r \in \mathbb{R} \setminus \{0\}$, A_r has the distribution given by (4.23).

By Naimark [7] (Remark 2, Chapter 19, p.90), it is not surprising that for A_r on $L^2(0,1)$ we always find discrete distributions. Then, we prove above theorem case by case.

4.2.1. *Dirichlet problem.* In the sequel the separation of variables method will be used several times. The idea is transforming the heat equation into second-order ordinary differential equations, or so-called Sturm-Liouville problem (see [10], Sect.5.3, p.105). Now, suppose the solution $u(t,x)$ can be written as the product of two parts

$$u(t,x) = T(t) \cdot X(x)$$

Then (4.7) implies

$$T'(t) \cdot X(x) = T(t) \cdot X''(x)$$

Assume $X(x)$ and $T(t)$ do not equals to zero on a positive measure set, then

$$\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)}$$

Since the right-hand side depends only on x and the left-hand side only on t, both sides should equal to some constant value $k \in \mathbb{C}$. Therefore, the problem transforms to solving following ordinary differential equation system:

$$T'(t) = kT(t), \quad X''(x) = kX(x) \tag{4.10}$$

Then, the boundary condition (4.5) becomes $X(0) = X(1) = 0$. When $k \neq 0$, the solution of the second equation in (4.10) should be in the form

$$X(x) = c_1 \mathrm{e}^{\zeta x} + c_2 \mathrm{e}^{-\zeta x} \tag{4.11}$$

where ζ is a square root of k. The boundary condition $X(0) = X(1) = 0$ implies $c_1 = -c_2 =: c$ and

$$\zeta = n\pi\mathrm{i} \tag{4.12}$$

is purely imaginary. So $k = -n^2\pi^2$ and $X(x) = 2c\mathrm{i} \cdot \sin(n\pi x)$. On the other hand, for the first equation in (4.10), we have $T(t) = \exp\{-n^2\pi^2 t\}$. By the superposition principle we know the solution should be

$$u(t,x) = \sum_{n=1}^{\infty} c_n \cdot \mathrm{e}^{-n^2\pi^2 t} \cdot \sin(n\pi x) \tag{4.13}$$

But $u(t,x)$ should be also compatible with the initial datum $u(x)$ as $t \to 0$. One may observe that $\{\sin(n\pi x)\}_{n\geq 1}$ forms an orthogonal basis in $L^2(0,1)$. Thus, the coefficients in (4.13) are

$$c_n = \frac{1}{\|\sin(n\pi x)\|^2} \int_0^1 u(x)\sin(n\pi x)\mathrm{d}x = 2\int_0^1 u(x)\sin(n\pi x)\mathrm{d}x$$

Therefore,

$$
\begin{aligned}
\left\langle \mathbb{1}, \mathrm{e}^{-tA_\infty}\mathbb{1}\right\rangle &= 2\sum_{n=1}^{\infty}\left[\int_0^1 \sin(n\pi x)\mathrm{d}x\cdot \mathrm{e}^{-n^2\pi^2 t}\cdot \int_0^1 \sin(n\pi x)\mathrm{d}x\right]\\
&= \sum_{n=1}^{\infty}\frac{2}{n^2\pi^2}(1-\cos(n\pi))^2\mathrm{e}^{-n^2\pi^2 t}\\
&= \sum_{n=0}^{\infty}\frac{8}{(2n+1)^2\pi^2}\cdot \mathrm{e}^{-(2n+1)^2\pi^2 t} \qquad (4.14)
\end{aligned}
$$

Applying the inverse Laplace transform on (4.14), we find the distribution of A_∞ with respect to the state $\mathbb{1}$

$$
\sum_{n=0}^{\infty}\frac{8}{(2n+1)^2\pi^2}\cdot\delta_{(2n+1)^2\pi^2}
$$

which is exactly (4.8). It is well-known that

$$
\sum_{n=0}^{\infty}\frac{8}{(2n+1)^2\pi^2} = 1
$$

One will see, that we use a similar idea to deal with Neumann problem and Robin problem.

4.2.2. *Neumann problem.* Now the system (4.10) remains the same. When $k=0$ there is only the trivial solution. When $k\neq 0$, we have (4.11), i.e. $X(x) = c_1\mathrm{e}^{\zeta x}+c_2\mathrm{e}^{-\zeta x}$. The Neumann boundary condition gives

$$
\zeta = (n+1/2)\,\pi\mathrm{i} \qquad (4.15)
$$

so $k=-(n+1/2)^2\pi^2$. Then, $X(x)=2c\mathrm{i}\cdot\sin((n+1/2)\pi x)$. For $T(t)$, we get $T(t)=\exp\{-(n+1/2)^2\pi^2 t\}$. By the principle of superposition, we obtain $u(t,x)$. Let $t=0$, use the initial value $u(x)$ to determine the coefficients. Observe that $\{\sin(n+1/2)\pi x\}_{n\geq 0}$ is an orthogonal basis in $L^2(0,1)$, so the solution should be

$$
u(t,x) = \sum_{n=0}^{\infty} c_n\cdot \mathrm{e}^{-(n+1/2)^2\pi^2 t}\cdot\sin((n+1/2)\pi x) \qquad (4.16)
$$

where

$$
\begin{aligned}
c_n &= \frac{1}{\|\sin((n+1/2)\pi x)\|^2}\int_0^1 u(x)\sin((n+1/2)\pi x)\mathrm{d}x\\
&= 2\int_0^1 u(x)\sin((n+1/2)\pi x)\mathrm{d}x
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\left\langle \mathbb{1}, \mathrm{e}^{-tA_0}\mathbb{1} \right\rangle &= 2\sum_{n=0}^{\infty}\left[\left(\int_0^1 \sin((n+1/2)\pi x)dx\right)^2 \cdot \mathrm{e}^{-(n+1/2)^2\pi^2 t}\right] \\
&= \sum_{n=0}^{\infty}\frac{2}{(n+1/2)^2\pi^2}\cdot \mathrm{e}^{-(n+1/2)^2\pi^2 t} \qquad (4.17)
\end{aligned}
$$

Implementing the inverse Laplace transform on (4.17), we find the distribution of A_0 with respect to the state $\mathbb{1}$

$$
\sum_{n=0}^{\infty}\frac{2}{(n+1/2)^2\pi^2}\cdot \delta_{(n+1/2)^2\pi^2}.
$$

This proves (4.9). It is also easy to verify that

$$
\sum_{n=0}^{\infty}\frac{2}{(n+1/2)^2\pi^2} = 1
$$

4.2.3. *Robin problem.* After separation of variable, the boundary conditions are

$$
X(0) = 0, \quad X'(1) + rX(1) = 0 \qquad (4.18)
$$

When $k = 0$, one gets only trivial solution. When $k \neq 0$, again there will be (4.11), i.e. $X(x) = c_1\mathrm{e}^{\zeta x} + c_2\mathrm{e}^{-\zeta x}$, where $\zeta \in \mathbb{C}$ is the complex square root of k. Then, (4.18) implies $c_1 = -c_2 =: c$, and $c(\zeta + r)\mathrm{e}^{\zeta} + c(\zeta - r)\mathrm{e}^{-\zeta} = 0$. Writing $\zeta = a + b\mathrm{i}$, where $a, b \in \mathbb{R}$, we have (when $r \neq \zeta$)

$$
\frac{r + (a + b\mathrm{i})}{r - (a + b\mathrm{i})}\cdot \mathrm{e}^{2a} = \mathrm{e}^{-2b\mathrm{i}}
$$

which is equivalent to the following system

$$
\frac{r^2 - a^2 - b^2}{(r-a)^2 + b^2}\cdot \mathrm{e}^{2a} = \cos 2b, \quad \frac{-2br}{(r-a)^2 + b^2}\cdot \mathrm{e}^{2a} = \sin 2b \qquad (4.19)
$$

Notice the natural condition $\sin^2 2b + \cos^2 2b = 1$ holds for all $b \in \mathbb{R}$, no matter what value does a have. Then, fix $a \in \mathbb{R}$ and let $b \to \infty$, we have

$$
\lim_{b\to\infty}\left(\sin^2 2b + \cos^2 2b\right) = \lim_{b\to\infty}\frac{(r^2 - a^2 - b^2)^2 + 4b^2r^2}{\left((k-a)^2 + b^2\right)^2}\cdot \mathrm{e}^{4a} = \mathrm{e}^{4a} = 1
$$

which compels $a = 0$. So $\zeta = b\mathrm{i}$ must be purely imaginary. Recalling the basic triangular formula $\tan\theta = \sin 2\theta / (1 + \cos 2\theta)$, (4.19) gives

$$
\tan b = -\frac{b}{r} \qquad (4.20)
$$

Notice that (4.20) gives only implicit solutions, and we shall denote the positive solutions by b_n, such that $0 < b_1 < b_2 < b_3 < \cdots$. Therefore, we have $X(x) = 2c\mathrm{i}\cdot\sin bx$. Combining $T(t)$ and $X(x)$, we get

$$
u_n(x,t) = c\cdot \mathrm{e}^{-b_n^2 t}\cdot \sin b_n x
$$

where b_n is the n-th positive solution of $\tan b = -b/r$. By the superposition principle, one knows

$$u(x,t) = \sum_{n=1}^{\infty} u_n(x,t) = \sum_{n=1}^{\infty} c_n \cdot \mathrm{e}^{-b_n^2 t} \cdot \sigma_n \sin(b_n x) \tag{4.21}$$

is also a solution, in which $\sigma_n := \|\sin(b_n x)\|^{-1}$ is the normalization constant. Now, we let $t = 0$ and use the initial datum to determine the constant c_n. Functions $\sin(b_n x)$ and $\sin(b_m x)$ are orthogonal whenever $n \neq m$, and c_n is determined by

$$c_n = \langle u(x), \sigma_n \sin b_n x\rangle = \sigma_n \int_0^1 u(x) \sin b_n x$$

Therefore, by (4.21), we know

$$\begin{aligned} \left\langle \mathbb{1}, \mathrm{e}^{-tA_r}\mathbb{1}\right\rangle &= \int_0^1 \mathbb{1}(x) \cdot \left(\sum_{n=1}^{\infty} \sigma_n^2 \int_0^1 \mathbb{1}(x) \sin b_n x \cdot \mathrm{e}^{-b_n^2 t} \cdot \sin b_n x \right) \mathrm{d}x \\ &= \sum_{n=1}^{\infty} \langle \mathbb{1}(x), \sigma_n \sin b_n x\rangle^2 \, \mathrm{e}^{-b_n^2 t} \end{aligned} \tag{4.22}$$

Thus, when $r \in \mathbb{R} \setminus \{0\}$, the inverse Laplace transform on (4.22) gives the distribution of A_r with respect to the state $\mathbb{1}$

$$\sum_{n=1}^{\infty} \langle \mathbb{1}(x), \sigma_n \sin b_n x\rangle^2 \cdot \delta_{b_n^2} \tag{4.23}$$

where b_n is the n-th positive solution of (4.20). Also, we notice that

$$\sum_{n=1}^{\infty} \langle \mathbb{1}(x), \sigma_n \sin b_n x\rangle^2 = 1 \tag{4.24}$$

since $\{\sigma_n \sin b_n x\}_{n\geq 1}$ is an orthonormal basis in $L^2(0,1)$.

We finish this paper by the following corollary, which gives additional properties of distributions of A_r on $L^2(0,1)$ with respect to state $\mathbb{1}$.

Corollary 4.2. *Let μ_r be the probability measure (4.8) when $r = \infty$, (4.9) when $r = 0$, (4.23) when $r \in \mathbb{R} \setminus \{0\}$. For $r \in \mathbb{R} \cup \{\infty\}$,*

1. *μ_r does not have first-order moment,*
2. *If $r \neq r'$ then μ_r is not absolutely continuous with respect to $\mu_{r'}$,*
3. *The map $r \mapsto \mu_r$ is continuous with respect to the weak topology on probability measures.*

Proof. The first two statements are obvious. For the third one, we need the fact that the distributions converge in weak topology if their corresponding Laplacian transforms converge pointwisely ([6] Ch.XIII, Sect.1, Th.2, p.431). In our case, when $r \to \infty$, the n-th solution of equation (4.20) $b_n \to n\pi$, this holds for all $n \geq 1$. Recall that $n\pi$ coincides with (4.12), i.e. the parameter inside the sine function in Dirichlet problem. On the other hand, no matter what value does r have, for fixed $t \geq 0$, $\exp\{-b_n^2 t\} \leq 1$. Considering also (4.24), we can observe that the sequence of summands in (4.22) is dominated by certain summable sequence in $l^1(\mathbb{R})$. Therefore, by dominated convergence theorem, we get the pointwise convergence (with respect to parameter t) of Laplacian transforms, then the convergence of probability measures in the weak topology comes out immediately. When $r \to 0$, the proof follows the same routine. $\square$

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Franco Fagnola: Department of Mathematics, Politecnico di Milano, Milan, 20133, Italy

E-mail address: `franco.fagnola@polimi.it`

Zheng Li: Department of Mathematics, Politecnico di Milano, Milan, 20133, Italy

E-mail address: `zheng.li@polimi.it`