Homework 2, Mathematics of Quantum Mechanics

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1 Kinetic Energy on the Open Interval

1.1 Preliminaries

Consider the operator $H = -\Delta$ on $C_c^\infty((0, 2\pi))$ and the (separable) Hilbert space $L^2((0, 2\pi))$. We start with some preliminaries: by definition,

$$\mathcal{D}(H^*) = \left\{ \phi \in L^2((0, 2\pi)) \mid \sup_{\psi \in \mathcal{H}, \|\psi\|=1} |\langle \phi | H\psi \rangle| < \infty \right\}$$

Indeed, for symmetric H,

$$\langle \phi | H\psi \rangle = \int_0^{2\pi} (-\Delta\phi)^* \psi \, d\mu \leq \| - \Delta\phi\|_2 \|\psi\|_2 = \|H\phi\|_2 \|\psi\|_2 \quad \text{on } (0, 2\pi)$$

Hence, we search for $\phi \in H^2((0, 2\pi))$

Remark: H is symmetric for $\phi \in H^2((0, 2\pi))$. In fact, when $\psi \in C_c^\infty((0, 2\pi))$,

$$\langle \phi | H\psi \rangle = -\phi^* \nabla\psi \Big|_0^{2\pi} + \nabla\phi^* \psi \Big|_0^{2\pi} + \langle H\phi | \psi \rangle = \langle H\phi | \psi \rangle$$

Note also that $C_c^\infty((0, 2\pi))$ is not dense in $H^1((0, 2\pi))$, whereas $C_c^\infty([0, 2\pi])$ is.

At this point, we already know that $\mathcal{D}(H^*) \subset H^2((0, 2\pi))$. This domain can slightly change if we change $\mathcal{D}(H)$. For instance, consider the o.n.c.s formed by the sequence $\left\{ \frac{e^{ikx}}{\sqrt{2\pi}} \right\}_{k \in \mathbb{Z}}$ on $L^2((0, 2\pi))$. Indeed, for $\phi \in L^2((0, 2\pi))$, we can write its Fourier expansion as follows:

$$\phi = \sum_{k \in \mathbb{Z}} \phi_k \frac{e^{ikx}}{\sqrt{2\pi}}$$

where $\phi_k =< e_k | \phi >$.

Remark: the span of this o.n.c.s. in finite.

Recall the Sobolev embedding $H^1((0,2\pi)) \hookrightarrow C^0((0,2\pi))$. Thus, whenever expanding a vector of $L^2((0,2\pi))$ on the previously mentioned basis, we get by continuity $\phi(0) = \phi(2\pi)$. The same holds also for $\nabla\phi$, which is indeed in $H^1((0,2\pi))$ and so the embedding still makes sense. Thus,

$$\mathcal{D}(H_0^*) \subset \left\{ \phi \in H^2((0,2\pi)) \;\middle|\; \phi(0) = \phi(2\pi), \nabla\phi(0) = \nabla\phi(2\pi) \right\}$$

1.2 On the domain of $-\Delta$

1. Take $\psi \in C^2([0,2\pi])$. Then, both ψ and its gradient belong to $C^0((0,2\pi)) \subset L^2((0,2\pi))$. This is enough to get $\psi \in \mathcal{D}(H^*)$. Furthermore, recall the alternative definition of Sobolev spaces of order p on intervals:

$$H^p((0,2\pi)) = \left\{ \psi \in L^2((0,2\pi)) \;\middle|\; \left((n^2+1)^{\frac{p}{2}}\psi_n\right)_{n\in\mathbb{Z}} \in \ell^2(\mathbb{Z}) \right\}$$

Thus, whenever we expand on the basis $\left\{\frac{e^{ikx}}{\sqrt{2\pi}}\right\}_{k\in\mathbb{Z}}$, we see immediately that

$$\left\{ \psi = \sum_{k\in\mathbb{Z}} \psi_k \mathrm{e}_k \;\middle|\; \{k^2\psi_k\} \in \ell^2(\mathbb{Z}) \right\} \subset \mathcal{D}(H_0^*)$$

Note that we get the additional boundary conditions for vectors of $\mathcal{D}(H_0^*)$ thanks to the chosen basis on which we consider all the Fourier expansions. Without explicitly fixing that basis, we only know that $\mathcal{D}(H^*) = H^2((0,2\pi))$. In this case, the fact that both $C^2([0,2\pi])$ and H^2 defined through sequences are subset of $\mathcal{D}(H^*)$ is trivial: in both cases we have that the norm of the laplacian is finite.

2. H is not essentially self-adjoint on $C_c^\infty((0,2\pi)) \subsetneq H^2((0,2\pi))$ because it is not closed there. Take $\psi_n \subset C_c^\infty((0,2\pi))$ such that $\psi_n \longrightarrow \psi \in L^2((0,2\pi))$ and $H\psi_n \longrightarrow \phi \in L^2((0,2\pi))$. Then $\psi_n \longrightarrow \psi$ in H^2. By Sobolev embedding, $H^2 \hookrightarrow L^\infty((0,2\pi))$, $\exists c > 0$ such that

$$\|\psi_n - \psi\|_\infty \le c\|\psi_n - \psi\|_{H^2}$$

Namely, $\psi_n \longrightarrow \psi$ uniformly a.e. in $(0,2\pi)$, which implies pointwise a.e. convergence. But ψ_n is a family of compactly supported functions, so pointwise convergence implies $\psi(0) = \psi(2\pi) = 0$. Thus,

$$\mathcal{D}(H) \subsetneq \mathcal{D}(\overline{H}) \subset H_0^2((0,2\pi)) \subsetneq \mathcal{D}(H^*) = H^2((0,2\pi))$$

And so, H is not essentially self-adjoint. However, since it is symmetric and bounded from below on its domain, it admits a self-adjoint extension (Friedrich's extension).

Remark: (*Positivity*) for $\psi \in C_c^\infty((0,2\pi))$, we have

$$\langle \psi | -\Delta\psi \rangle = \int_0^{2\pi} |\nabla\psi|^2 \, d\mu \geq 0$$

Remark: The domain of $\overline{H}$ (for H defined on smooth functions with compact support) is

$$\mathcal{D}(\overline{H}) = \left\{ \psi \in H^2((0,2\pi)) \,\middle|\, \psi(0) = \psi(2\pi) = 0, \nabla\psi(0) = \nabla\psi(2\pi) = 0 \right\}$$

3. We now look for (explicit) families of self-adjoint extensions of H. To preserve symmetry, we need to restrict $H^2((0,2\pi))$. In particular, we need the following identity to be true for all vectors in the domain:

$$\nabla\phi^*(2\pi)\psi(2\pi) - \nabla\phi^*(0)\psi(0) + \phi^*(0)\nabla\psi(0) - \phi^*(2\pi)\nabla\psi(2\pi) = 0$$

For generic $\psi \in H^2((0,2\pi))$ we observe that the dimension of both the deficiencies spaces $\mathcal{H}_\pm$ is 2 (see point 4 and do not apply boundary conditions a posteriori). Therefore, we already know that the number of parameters characterizing the family of self-adjoint extensions must be 2. An explicit form for the family of self-adjoint extensions require some effort. Here we refer to a result which can be found in [1]. The different extensions for the free kinetic energy on $\Omega = (0,2\pi)$ are parameterized by 2 x 2 unitary matrices as follows:

$$\begin{pmatrix} \Phi(0) + i\nabla\Phi(0) \\ \Phi(2\pi) - i\nabla\Phi(2\pi) \end{pmatrix} = U \begin{pmatrix} \Phi(0) - i\nabla\Phi(0) \\ \Phi(2\pi) + i\nabla\Phi(2\pi) \end{pmatrix}$$

In the special case in which

$$U = \begin{pmatrix} e^{i\epsilon} & 0 \\ 0 & e^{i\gamma} \end{pmatrix}$$

we get the boundary conditions

$$-\sin\frac{\epsilon}{2}\Phi(0) + \cos\frac{\epsilon}{2}\nabla\Phi(0) = 0$$

$$-\sin\frac{\gamma}{2}\Phi(2\pi) - \cos\frac{\gamma}{2}\nabla\Phi(2\pi) = 0$$

For $\epsilon = 0$, $\gamma = 0$ we are imposing Neumann boundaries, whereas for $\epsilon = \pi$, $\gamma = \pi$ Dirichlet boundaries. By this fact, it follows immediately that H_N and H_D belongs to this family.

Remark: Unitary 2 x 2 matrices span over two dimensional vector spaces. This explain why the family is characterized by exactly 2 parameters.

4. H_N, H_D with domains $\mathcal{D}(H_N)$, $\mathcal{D}(H_D)$ respectively are *closed* (we deduce

it by previous point) symmetric operators. Moreover, they are bounded from below (see prevoius remarks).
Obviously, they both admit a self-adjoint extension. Here we show another way to find that they are self-adjoint on their domains exploiting directly Von Neumann theory of self-adjoint extensions. First of all, observe that those domains are quite similar: in fact, they impose an 'equivalent' condition on the H^2 vector ψ with respect to the quadratic form induced by the scalar product $< \phi | H\psi >$, with $\phi \in \mathcal{D}_H$. Now, the (weak) solutions of the deficiency equations are trivially given by

$$\psi_{\mp}(x) = c_1 e^{(1\pm i)\frac{x}{\sqrt{2}}} + c_2 e^{-(1\pm i)\frac{x}{\sqrt{2}}}$$

where c_1, c_2 are real numbers and $x \in (0, 2\pi)$. By simple computations, we observe that, as a consequence of the boundary condition $\psi(0) = \psi(2\pi) = 0$ and $\nabla\psi(0) = \nabla\psi(2\pi) = 0$, for $\mathcal{D}(H_N)$ and $\mathcal{D}(H_D)$ respectively, $\psi_{\mp}$ must be identically zero. Hence the deficiency spaces have dimension zero. By Von Neumann theorem on self-adjoint extensions we get that the kinetic energy is self-adjoint on those domains.

2 Small Perturbations of the Free Hamiltonian

5. Recall that the operator $U : L^2((0, 2\pi)) \longrightarrow \ell^2(\mathbb{Z})$ which maps ψ onto its Fourier coefficient is unitary and that for $\psi \in H^2((0, 2\pi))$ the norms $\|\Delta\psi\|$ and $\|\{k^2\psi_k\}_{k\in\mathbb{Z}}\|$ are equivalent (it follows by the definition of H^2 on intervals). For the sake of completeness, we rewrite $\mathcal{D}(H_N)$, $\mathcal{D}(H_D)$ in terms of their Fourier coefficients:

$$\mathcal{D}(H_D) = \left\{ \psi \in H^2((0, 2\pi)) \;\middle|\; \{n^2\psi_n\} \in \ell^2(\mathbb{Z}), \sum_{n\in\mathbb{Z}} \psi_n = 0 \right\}$$

$$\mathcal{D}(H_N) = \left\{ \psi \in H^2((0, 2\pi)) \;\middle|\; \{n^2\psi_n\} \in \ell^2(\mathbb{Z}), \sum_{n\in\mathbb{Z}} n\psi_n = 0 \right\}$$

Now, we exploit the abstract Fourier transform for Hilbert spaces:

$$\|\psi\|_\infty \le \sum_{k\in\mathbb{Z}} \|\psi_k e_k\|_\infty \le c \sum_{k\in\mathbb{Z}} |\psi_k| \le c \sum_{k\in\mathbb{Z}} |\psi_k| \, \frac{k^2 + \lambda}{k^2 + \lambda} = (*)$$

for $c > 0$, $\lambda > 0$. Consider now the measure space $(\mathbb{Z}, \mathcal{P}(\mathbb{Z}), \mu_c)$. By Hölder inequality,

$$\begin{aligned}
(*) &\le c \left(\sum_{k\in\mathbb{Z}} \frac{1}{(k^2 + \lambda)^2} \right)^{\frac{1}{2}} \|\{(k^2 + \lambda)\psi_k\}\|_{\ell^2} \\
&\le c' \left(\frac{1}{\lambda^{\frac{1}{4}}} \|\{k^2\psi_k\}\|_{\ell^2} + \lambda^{\frac{3}{4}} \|\{\psi_k\}\|_{\ell^2} \right) \\
&\le c'' \frac{1}{\lambda^{\frac{1}{4}}} \|\{k^2\psi_k\}\|_{\ell^2} + c'\lambda^{\frac{3}{4}} \|\{\psi_k\}\|_{\ell^2}
\end{aligned}$$

for suitable c', $c'' > 0$. Thus, we get the following Sobolev inequality: for all $\psi \in H^2((0, 2\pi))$ and for all $a > 0$, there exists $b < \infty$ such that

$$\|\psi\|_\infty \leq a\| - \Delta\psi\|_2 + b\|\psi\|_2$$

6. We decompose the potential as follows:

$$V(x) = \frac{1}{x^{1/4}} = \frac{1}{x^{1/4}}\chi_{(0,K]}(x) + \frac{1}{x^{1/4}}\chi_{[K,2\pi)}(x)$$

where $K \in (\epsilon, 2\pi - \epsilon)$, $\epsilon > 0$. But then, $V \in L^2((0, 2\pi)) + L^\infty((0, 2\pi))$. Let us define

$$V_1(x) := \frac{1}{x^{1/4}}\chi_{(0,K]}(x)$$

and

$$V_2(x) := \frac{1}{x^{1/4}}\chi_{[K,2\pi)}(x)$$

For $\psi \in \mathcal{D}(H_{N/D})$, it holds that

$$\begin{aligned}\|V\psi\|_2 \leq \|V_1\psi\|_2 + \|V_2\psi\|_2 &\leq \|V_1\|_2\|\psi\|_\infty + \|V_2\|_\infty\|\psi\|_2 \\ &\leq a\|V_1\|_2\| - \Delta\psi\|_2 + b\|V_1\|_2\|\psi\|_2 + \|V_2\|_\infty\|\psi\|_2 \\ &= a\|V_1\|_2\|H\psi\|_2 + b(\|V_1\|_2 + \|V_2\|_\infty)\|\psi\|_2\end{aligned}$$

Remark: The domain of self-adjointness of V is clearly larger that $\mathcal{D}(H_{N/D})$.

Therefore, V is Kato-small w.r.t. H on $\mathcal{D}(H_{N/D})$, on which H is self-adjoint. By Kato theorem on small perturbations of self-adjoint operators, we get that both $H_N + V$ and $H_D + V$ are self-adjoints operators on their domains.

References

[1] M. ASOREY, A. IBORT, and G. MARMO. "GLOBAL THEORY OF QUANTUM BOUNDARY CONDITIONS AND TOPOLOGY CHANGE". In: *International Journal of Modern Physics A* 20.05 (Feb. 2005), pp. 1001–1025. ISSN: 1793-656X. DOI: 10.1142/s0217751x05019798. URL: http://dx.doi.org/10.1142/S0217751X05019798.