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Second correction

University of Toronto
Department of Mathematics

Solution to Test 3
Differential Equations of Mathematical Physics
(APM 351 Y)

Max Lein

20 March 2014, 09:10–10:50, Sidney Smith Hall, SS 1074

Remarks:
Please verify the completeness of the exam: **6** problems

Time allotted: **100** minutes

Allowed aids: **none**

1. **The framework of quantum mechanics (12 points)**

Consider a quantum particle moving in $\mathbb{R}^d$.

(i) Give an example of a Schrödinger operator. Explain the physical meaning of each of the terms.

(ii) State the Schrödinger equation.

(iii) Give the notion of observable, state and dynamical equation.

(iv) Show that $H = H^*$ implies $\left\|\mathrm{e}^{-\mathrm{i}tH}\psi\right\|^2 = \|\psi\|^2$ for all $t \in \mathbb{R}$.

(v) Explain the significance of (iv) for the Born rule.

Solution:

(i) $H = -\Delta_x + V$ [1] where $-\Delta_x$ is the kinetic energy and V is the potential energy [1].

(ii) $\mathrm{i}\,\hbar\,\partial_t\psi(t) = H\psi(t)$, $\psi(0) = \psi_0 \in L^2(\mathbb{R}^d)$ where $\hbar$ is Planck's constant [1]

(iii) **Observables** are selfadjoint operators $F = F^*$ on $L^2(\mathbb{R}^d)$ with dense domain $\mathcal{D}(F)$. [1]

States are density operators ρ, i. e. operators which satisfy $\rho^* = \rho \geq 0$ [1] and $\mathrm{Tr}\,\rho = 1$ [1].

Dynamical equation: Heisenberg equation for observables:

$$\frac{\mathrm{d}}{\mathrm{d}t}F(t) = \frac{\mathrm{i}}{\hbar}\big[H, F(t)\big], \qquad F(0) = F \qquad [1]$$

Liouville equation for states:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\frac{\mathrm{i}}{\hbar}\big[H, \rho(t)\big], \qquad \rho(0) = \rho$$

(Giving one dynamical equation suffices. Also the Schrödinger equation is accepted as solution. $\hbar$ need not be present to get full points.)

(iv) At $t = 0$, clearly $\left\|\mathrm{e}^{-\mathrm{i}tH}\psi\right\|^2\big|_{t=0} = \|\psi\|^2 = 1$ [1], and since the time-derivative vanishes,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left\|\mathrm{e}^{-\mathrm{i}tH}\psi\right\|^2 &\overset{[1]}{=} \big\langle -\mathrm{i}H\,\mathrm{e}^{-\mathrm{i}tH}\psi, \mathrm{e}^{-\mathrm{i}tH}\psi\big\rangle + \big\langle \mathrm{e}^{-\mathrm{i}tH}\psi, -\mathrm{i}H\,\mathrm{e}^{-\mathrm{i}tH}\psi\big\rangle \\ &= \mathrm{i}\,\big\langle \mathrm{e}^{-\mathrm{i}tH}\psi, \big(H^* - H\big)\mathrm{e}^{-\mathrm{i}tH}\psi\big\rangle \overset{[1]}{=} 0,\end{aligned}$$

$\left\|\mathrm{e}^{-\mathrm{i}tH}\psi\right\|^2 = \|\psi\|^2$ holds for all $t \in \mathbb{R}$ [1].

(v) The Born rule states that $\left|\psi(t,x)\right|^2$ is a probability density in $\mathbb{R}^d$, so the physical interpretation of (iv) is the conservation of probability. [1]

2. **The Birman-Schwinger principle (6 points)**

Consider the Schrödinger operator $H = -\Delta_x + V$ on $\mathbb{R}^d$ where $V \leq 0$ is a non-positive potential which decays at ∞, $\lim_{|x|\to\infty} V(x) = 0$.

(i) Give the Birman-Schwinger operator K_E and state the Birman-Schwinger principle.

(ii) Give a sufficient condition on K_E for the absence of eigenvalues of H at $-E < 0$.

Solution:

(i) The Birman-Schwinger operator is defined as

$$K_E = |V|^{1/2} \left(-\Delta_x + E\right)^{-1} |V|^{1/2}. \qquad [2]$$

The Birman-Schwinger principle states H has an eigenvalue at $-E$, $E > 0$, if and only if the Birman-Schwinger operator K_E has an eigenvalue at 1. [2]

(ii) For instance, if $\|K_E\| < 1$ [1] then K_E cannot have an eigenvalue at 1, and thus by the Birman-Schwinger principle H cannot have an eigenvalue at $-E$ [1].

3. **Green's functions for $-\partial_x^2 + E$ (14 points)**

Consider the linear operator $L_E := -\partial_x^2 + E$ for $E > 0$ on $\mathbb{R}$. Define the function

$$R_E(x) := \frac{\mathrm{e}^{-\sqrt{E}\,|x|}}{2\sqrt{E}}.$$

(i) Compute $\big(-\partial_x^2 + E\big) R_E(x)$ in the sense of tempered distributions.

(ii) Find the Green's function $G(x, y)$ to the operator L_E.

(iii) Given $\varphi \in L^2(\mathbb{R})$, solve $L_E \psi = \varphi$ for ψ.

Solution:

(i) Let us first compute the second weak derivative of R_E: for any $\varphi \in \mathcal{S}(\mathbb{R})$, we compute

$$\begin{aligned}
(-\partial_x^2 R_E, \varphi) &\overset{[1]}{=} -\big(R_E, \partial_x^2 \varphi\big) \overset{[1]}{=} -\int_{-\infty}^{0} \mathrm{d}x\, \frac{\mathrm{e}^{+\sqrt{E}\,x}}{2\sqrt{E}}\, \partial_x^2 \varphi(x) - \int_{0}^{+\infty} \mathrm{d}x\, \frac{\mathrm{e}^{-\sqrt{E}\,x}}{2\sqrt{E}}\, \partial_x^2 \varphi(x) \\
&\overset{[2]}{=} -\left[\frac{\mathrm{e}^{+\sqrt{E}\,x}}{2\sqrt{E}}\, \partial_x \varphi(x)\right]_{-\infty}^{0} + \int_{-\infty}^{0} \mathrm{d}x\, \frac{1}{2}\, \mathrm{e}^{+\sqrt{E}\,x}\, \partial_x \varphi(x) + \\
&\qquad - \left[\frac{\mathrm{e}^{-\sqrt{E}\,x}}{2\sqrt{E}}\, \partial_x \varphi(x)\right]_{0}^{+\infty} - \int_{0}^{+\infty} \mathrm{d}x\, \frac{1}{2}\, \mathrm{e}^{-\sqrt{E}\,x}\, \partial_x \varphi(x) \\
&\overset{[2]}{=} -\frac{\partial_x \varphi(0)}{2\sqrt{E}} + \frac{\partial_x \varphi(0)}{2\sqrt{E}} + \Big[\tfrac{1}{2} \mathrm{e}^{+\sqrt{E}\,x}\, \varphi(x)\Big]_{-\infty}^{0} - \int_{-\infty}^{0} \mathrm{d}x\, \frac{\sqrt{E}}{2}\, \mathrm{e}^{+\sqrt{E}\,x}\, \varphi(x) + \\
&\qquad - \Big[\tfrac{1}{2} \mathrm{e}^{-\sqrt{E}\,x}\, \varphi(x)\Big]_{0}^{+\infty} - \int_{0}^{+\infty} \mathrm{d}x\, \frac{\sqrt{E}}{2}\, \mathrm{e}^{-\sqrt{E}\,x}\, \varphi(x) \\
&\overset{[2]}{=} \varphi(0) - E \int_{\mathbb{R}} \mathrm{d}x\, \frac{\mathrm{e}^{-\sqrt{E}\,|x|}}{2\sqrt{E}}\, \varphi(x) \overset{[1]}{=} \big(\delta - E\, R_E, \varphi\big),
\end{aligned}$$

and hence, L_E applied to R_E yields

$$\big(-\partial_x^2 + E\big) R_E \overset{[1]}{=} \delta - E\, R_E + E\, R_E \overset{[1]}{=} \delta.$$

(ii) The Green's function is $G(x, y) := R_E(x - y)$ because $L_E G(x, y) = \delta(x - y)$ by (i) [2].

(iii) The solution to $L_E u = f$ is given by

$$u(x) = \int_{\mathbb{R}} \mathrm{d}x\, G(x, y)\, f(y) = R_E * f(x). \qquad [1]$$

4. **Symmetric operators (4 points)**

Show that $H = -\partial_x^2$ is symmetric on

$$\mathcal{D} := \big\{\psi \in \mathcal{C}^2([0,1]) \;\mid\; \varphi(0) = 0 = \varphi(1)\big\} \subset L^2([0,1]).$$

Solution:

Let $\varphi, \psi \in \mathcal{D}$.

$$\begin{aligned}
\langle \varphi, H\psi\rangle &\overset{[1]}{=} -\int_0^1 \mathrm{d}x\,\overline{\varphi(x)}\,\partial_x^2\psi(x) \\
&\overset{[1]}{=} -\underbrace{\Big[\overline{\varphi(x)}\,\partial_x\psi(x)\Big]_0^1}_{=0} + \int_0^1 \mathrm{d}x\,\overline{\partial_x\varphi(x)}\,\partial_x\psi(x) = \int_0^1 \mathrm{d}x\,\overline{\partial_x\varphi(x)}\,\partial_x\psi(x) \\
&\overset{[1]}{=} \underbrace{\Big[\overline{\partial_x\varphi(x)}\,\psi(x)\Big]_0^1}_{=0} - \int_0^1 \mathrm{d}x\,\overline{\partial_x^2\varphi(x)}\,\psi(x) \overset{[1]}{=} \langle H\varphi, \psi\rangle
\end{aligned}$$

5. **The quantum energy functional (15 points)**

Define the average energy

$$\mathcal{E}(\varphi) = \int_{\mathbb{R}} \mathrm{d}x \, \Bigl(\bigl| \partial_x \varphi(x) \bigr|^2 + V(x) \, \bigl| \varphi(x) \bigr|^2 \Bigr)$$

associated to the quantum hamiltonian $H = -\partial_x^2 + V$ and $\varphi \in \mathcal{S}(\mathbb{R})$ for the potential

$$V(x) = \begin{cases} -x & 0 \leq x \leq 1 \\ 0 & \text{else} \end{cases} . \tag{1}$$

Moreover, define the family of scaled Gaußians $\varphi_\lambda(x) := \pi^{-1/4} \sqrt{\lambda} \, \mathrm{e}^{-\frac{\lambda^2}{2} x^2}$ for $\lambda > 0$.

(i) Determine the expected value of the energy $E(\lambda) := \mathcal{E}(\varphi_\lambda)$.

(ii) Express $E(\lambda)$ as a power series in λ.

(iii) Use the quadratic approximation of $E(\lambda) = e_0 + \lambda \, e_1 + \lambda^2 \, e_2 + \mathcal{O}(\lambda^3)$ to minimize $E(\lambda)$ for small λ. Compute the minimum of $E(\lambda)$ up to $\mathcal{O}(\lambda^3)$.

(iv) Does this hamiltonian have a bound state? Justify your answer.

Hint: You may use $\bigl(\mathcal{F} \mathrm{e}^{-\frac{\lambda^2}{2} x^2}\bigr)(\xi) = \lambda^{-1} \, \mathrm{e}^{-\frac{\xi^2}{2\lambda^2}}$ and $\int_{\mathbb{R}} \mathrm{d}x \, \mathrm{e}^{-\lambda^2 x^2} = \frac{\sqrt{\pi}}{\lambda}$ where $\lambda > 0$.

Solution:

(i) We first compute the kinetic energy part:

$$\begin{aligned}
\int_{\mathbb{R}} \mathrm{d}x \, \bigl| \partial_x \varphi(x) \bigr|^2 &\overset{[1]}{=} \int_{\mathbb{R}} \mathrm{d}x \, \frac{\lambda}{\sqrt{\pi}} \Bigl(-\lambda^2 \, x \, \mathrm{e}^{-\frac{\lambda^2}{2} x^2} \Bigr)^2 = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{d}x \, \lambda^5 \, x^2 \, \mathrm{e}^{-\lambda^2 x^2} \\
&= \frac{\lambda^2}{\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{d}(\lambda x) \, (\lambda x)^2 \, \mathrm{e}^{-(\lambda x)^2} \overset{[1]}{=} \frac{\lambda^2}{\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{d}y \, y \cdot y \, \mathrm{e}^{-y^2} \\
&\overset{[1]}{=} \frac{\lambda^2}{\sqrt{\pi}} \biggl[-\frac{1}{2} y \, \mathrm{e}^{-y^2} \biggr]_{-\infty}^{+\infty} + \frac{\lambda^2}{2\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{-y^2} = \frac{\lambda^2}{2\sqrt{\pi}} \sqrt{\pi} \overset{[1]}{=} \frac{\lambda^2}{2}
\end{aligned}$$

The expectation value of the potential energy is

$$\begin{aligned}
\int_{\mathbb{R}} \mathrm{d}x \, V(x) \, \bigl| \partial_x \varphi(x) \bigr|^2 &\overset{[1]}{=} -\frac{1}{\sqrt{\pi}} \int_0^1 \mathrm{d}x \, \lambda \, x \, \mathrm{e}^{-\lambda^2 x^2} \overset{[1]}{=} -\frac{1}{\lambda \sqrt{\pi}} \int_0^1 \mathrm{d}(\lambda x) \, (\lambda x) \, \mathrm{e}^{-(\lambda x)^2} \\
&\overset{[1]}{=} +\frac{1}{\lambda \sqrt{\pi}} \Bigl[\tfrac{1}{2} \, \mathrm{e}^{-\lambda^2 x^2} \Bigr]_0^1 \overset{[1]}{=} \frac{1}{\lambda \, 2\sqrt{\pi}} \bigl(\mathrm{e}^{-\lambda^2} - 1 \bigr).
\end{aligned}$$

So overall, the energy expectation value with respect to φ_λ combines to

$$E(\lambda) \overset{[1]}{=} \frac{\lambda^2}{2} + \frac{1}{\lambda \, 2\sqrt{\pi}} \bigl(\mathrm{e}^{-\lambda^2} - 1 \bigr).$$

(ii) We plug in the exponential series and use that the first term of the series cancels:

$$\begin{aligned}
E(\lambda) &\overset{[1]}{=} \frac{\lambda^2}{2} + \frac{1}{\lambda \, 2\sqrt{\pi}} \left(\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \, \lambda^{2n} - 1 \right) \\
&\overset{[1]}{=} \frac{\lambda^2}{2} + \frac{1}{2\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \, \lambda^{2n-1} \\
&= \frac{\lambda^2}{2} - \frac{\lambda}{2\sqrt{\pi}} + \mathcal{O}(\lambda^3)
\end{aligned}$$

(iii) The derivative of E is

$$E'(\lambda) = \lambda - \tfrac{1}{2\sqrt{\pi}} + \mathcal{O}(\lambda^2) \stackrel{!}{=} 0. \qquad [1]$$

That means the critical point is approximately $\lambda_{\text{min}} \approx \frac{1}{2\sqrt{\pi}}$ [1]. Given that $E''(\lambda) = 1 + \mathcal{O}(\lambda) > 0$ this point is actually a minimum [1] and the energy at the critical energy is

$$E\big(\tfrac{1}{2\sqrt{\pi}}\big) \approx \frac{1}{8\pi} - \frac{1}{4\pi} = -\frac{1}{8\pi} \qquad [1]$$

up to errors of higher order.

(iv) $V \neq 0$ is a non-positive potential in one dimension. Then by Theorem 9.3.7, a bound state exists [1].

6. **The spectrum of an operator (5 points)**

Let T be a bounded operator on a Hilbert space $\mathcal{H}_1$ and $U : \mathcal{H}_1 \longrightarrow \mathcal{H}_2$ a unitary between two Hilbert spaces. Show $\sigma(T) = \sigma\big(U\,T\,U^{-1}\big)$.

Solution:

The spectrum $\sigma(T)$ is comprised of those $z \in \mathbb{C}$ for which $T - z$ is not invertible [1]. Since

$$\big(U\,(T-z)\,U^{-1}\big)^{-1} = \big(U^{-1}\big)^{-1}\,(T-z)^{-1}\,U^{-1} = U\,(T-z)^{-1}\,U^{-1} \qquad [1]$$

the operator $T - z$ is invertible if and only if $U\,T\,U^{-1} - z \overset{[1]}{=} U\,\big(T - z\big)\,U^{-1}$ is invertible [1]. Hence, $\sigma(T) = \sigma\big(U\,T\,U^{-1}\big)$ [1].