Modern Algebra

Chapter I. Basic Ideas of Hilbert Space Theory

I.5. Wave Mechanics of a Single Particle Moving in One Dimension—Proofs of Theorems

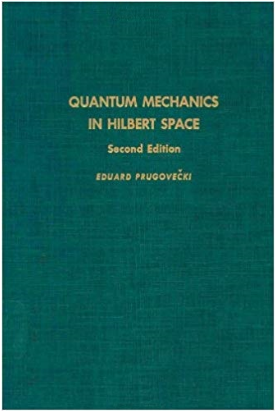

Table of contents

Theorem I.5.A

Theorem I.5.A. Schroedinger's equation implies that $\|\psi(x,t)\|$ is a constant with respect to time t where for each fixed t, $\lim_{x\to\pm\infty}\psi(x,t)=0$ and $\lim_{x\to\pm\infty}\left(\frac{\partial\psi(x,t)}{\partial x}\right)=0$.

Proof. We justify the claim by showing $\frac{d}{dt}[\|\psi(x,t)\|^2]=0$. We have

$$\begin{aligned}
\frac{d}{dt}[\|\psi(x,t)\|^2] &= \frac{d}{dt}\left[\int_{-\infty}^{\infty}|\psi(x,t)^2\,dx\right]=\frac{d}{dt}\left[\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)\,dx\right]\\
&= \int_{-\infty}^{\infty}\frac{\partial}{\partial t}[\psi^*(x,t)\psi(x,t)]\,dx \text{ by Leibniz's Rule}\\
&= \int_{-\infty}^{\infty}\left(\frac{\partial\psi^*(x,t)}{\partial t}\psi(x,t)+\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial t}\right)dx\\
&= \int_{-\infty}^{\infty}\left\{\left(\frac{\hbar}{2mi}\frac{\partial\psi^*(x,t)}{\partial x^2}-\frac{1}{i\hbar}V(x)\psi^*(x,t)\right)\psi(x,t)\right.\\
&\qquad \left.+\psi^*(x,t)\left(-\frac{\hbar}{2mi}\frac{\partial^2\psi(x,t)}{\partial x^2}+\frac{1}{i\hbar}V(x)\psi(x,t)\right)\right\}dx\ldots
\end{aligned}$$

Theorem I.5.A

Theorem I.5.A. Schroedinger's equation implies that $\|\psi(x,t)\|$ is a constant with respect to time t where for each fixed t, $\lim_{x\to\pm\infty}\psi(x,t)=0$ and $\lim_{x\to\pm\infty}\left(\frac{\partial\psi(x,t)}{\partial x}\right)=0$.

Proof. We justify the claim by showing $\frac{d}{dt}[\|\psi(x,t)\|^2]=0$. We have

$$\begin{aligned}
\frac{d}{dt}[\|\psi(x,t)\|^2] &= \frac{d}{dt}\left[\int_{-\infty}^{\infty}|\psi(x,t)^2\,dx\right]=\frac{d}{dt}\left[\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)\,dx\right]\\
&= \int_{-\infty}^{\infty}\frac{\partial}{\partial t}[\psi^*(x,t)\psi(x,t)]\,dx \text{ by Leibniz's Rule}\\
&= \int_{-\infty}^{\infty}\left(\frac{\partial\psi^*(x,t)}{\partial t}\psi(x,t)+\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial t}\right)\,dx\\
&= \int_{-\infty}^{\infty}\left\{\left(\frac{\hbar}{2mi}\frac{\partial\psi^*(x,t)}{\partial x^2}-\frac{1}{i\hbar}V(x)\psi^*(x,t)\right)\psi(x,t)\right.\\
&\qquad \left.+\psi^*(x,t)\left(-\frac{\hbar}{2mi}\frac{\partial^2\psi(x,t)}{\partial x^2}+\frac{1}{i\hbar}V(x)\psi(x,t)\right)\right\}\,dx\ldots
\end{aligned}$$

Theorem I.5.A (continued 1)

Proof (continued).

by the conjugate of Schroedinger's equation for $\dfrac{\partial \psi^*(x,t)}{\partial t}$

and Schroedinger's equation for $\dfrac{\partial \psi(x,t)}{\partial t}$

$$
\begin{aligned}
&= \frac{\hbar}{2mi}\int_{-\infty}^{\infty}\left(\frac{\partial^2\psi^*(x,t)}{\partial x^2}\psi(x,t) = \psi^*(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2}\right)\,dx \\
&= \frac{\hbar}{2mi}\int_{-\infty}^{\infty}\left(\frac{\partial^2\psi^*}{\partial x^2}\psi + \frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\partial\psi\partial x - \psi^*\frac{\partial^2\psi}{\partial x^2}\right)\,dx \\
&= \frac{\hbar}{2mi}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left[\frac{\partial\psi^*}{\partial x}\psi - \psi^*\frac{\partial\psi}{\partial x}\right]\,dx \\
&= \frac{\hbar}{2mi}\left(\frac{\partial\psi^*}{\partial x}\psi - \psi^*\frac{\partial\psi}{\partial x}\right)\Bigg|_{-\infty}^{\infty} \\
&= 0 \text{ since } \lim_{x\to\pm\infty}\psi(x,t) = \lim_{x\to\pm\infty}\frac{\partial\psi(x,t)}{\partial x} = 0.
\end{aligned}
$$

Theorem I.5.A (continued 2)

Theorem I.5.A. Schroedinger's equation implies that $\|\psi(x,t)\|$ is a constant with respect to time t where for each fixed t, $\lim_{x\to\pm\infty}\psi(x,t)=0$ and $\lim_{x\to\pm\infty}\left(\frac{\partial\psi(x,t)}{\partial x}\right)=0$.

Proof (continued). So $\frac{d}{dt}[\|\psi(x,t)\|^2]=0$ and $\|\psi(x,t)\|^2$ is a constant real valued continuous function of t. That is, $\|\psi(x,t)\|$ is constant with respect to t, as claimed. $\square$

Theorem I.5.1

Theorem I.5.1. If $\psi_1(x)$ and $\psi_2(x)$, their first derivatives $d\psi_1(x)/dx$ and $d\psi_2(x)/dx$, as well as $V(x)\psi_1(x)$ and $V(x)\psi_2(x)$ are from $\mathcal{C}^1_{(2)}(\mathbb{R})$, then

$$\left\langle \psi_1(x) \;\middle|\; -\frac{\hbar}{2m}\frac{d^2\psi_2(x)}{dx^2} + V(x)\psi_2(x) \right\rangle$$

$$= \left\langle -\frac{\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2} + V(x)\psi_1(x) \;\middle|\; \psi_2(x) \right\rangle.$$

In each solution $\psi(x)$ of the time-independent Schroedinger equation (5.7) has the property that $\psi(x), d\psi(x)/dx, V(x)\psi(x) \in \mathcal{C}^1_{(2)}(\mathbb{R})$, then each eigenvalue E of the time-independent Schroedinger equation is a real number, and if $\psi_1(x)$ and $\psi_2(x)$ are two eigenfunctions of the time-independent Schroedinger equation corresponding to two distinct eigenvalues $E_1 \neq E_2$, then $\psi_1(x)$ and $\psi_2(x)$ are orthogonal.

Theorem I.5.1 (continued 1)

Proof. We have (not writing the variable x):

$$\int_{-a}^{a} \psi_1^* \left(-\frac{\hbar^2}{2m} \frac{d^2\psi_2}{dx^2} + V\psi_2 \right) \, dx$$

$$\begin{aligned}
= & \int_{-a}^{a} -\frac{\hbar^2}{2m}\psi_1^* \frac{d^2\psi_2}{dx^2} \, dx + \int_{-a}^{a} V\psi_1^*\psi_2 \, dx \\
& \text{let } u = -\frac{\hbar^2}{2m}\psi_1^* \text{ and } dv = \frac{d^2\psi_2}{dx^2} dx \\
& \text{so } du = -\frac{\hbar^2}{2m}\frac{d\psi_1^*}{dx} dx \text{ and } v = \frac{d\psi_2}{dx} \\
= & -\frac{\hbar^2}{2m}\psi^* \frac{d\psi_2}{dx}\Big|_{-a}^{a} - \int_{-a}^{a} -\frac{\hbar^2}{2m}\frac{d\psi_1^*}{dx}\frac{d\psi_2}{dx} \, dx + \int_{-a}^{a} V\psi_1^*\psi_2 \, dx \ldots
\end{aligned}$$

Theorem I.5.1 (continued 2)

Proof (continued). . . .

$$= \quad -\frac{\hbar^2}{2m}\psi^*\frac{d\psi_2}{dx}\bigg|_{-a}^{a} - \int_{-a}^{a} -\frac{\hbar^2}{2m}\frac{d\psi_1^*}{dx}\frac{d\psi_2}{dx}\,dx + \int_{-a}^{a} V\psi_1^*\psi_2\,dx$$

$$\text{let } u = \frac{d\psi_1^*}{dx} \text{ and } dv = \frac{d\psi_2}{dx}\,dx$$

$$\text{so } du = \frac{d^2\psi_1^*}{dx^2}\,dx \text{ and } v = \psi_2$$

$$= \quad \left(-\frac{\hbar^2}{2m}\psi_1^*\frac{d\psi_2}{dx} + \frac{\hbar^2}{2m}\frac{d\psi_1^*}{dx}\psi_2\right)\bigg|_{-a}^{a}$$

$$-\frac{\hbar^2}{2m}\int_{-a}^{a}\psi_2\frac{d^2\psi_1^*}{dx^2}\,dx + \int_{-1}^{a} V\psi_1^*\psi_2\,dx$$

$$= \quad -\frac{\hbar^2}{2m}\left(\psi_1^*\frac{d\psi_2}{dx} - \frac{d\psi_1^*}{dx}\psi_2\right)\bigg|_{-a}^{a} + \int_{-a}^{a}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi_1^*}{dx^2} + V\psi_1^*\right)\psi_2\,dx.$$

Theorem I.5.1 (continued 3)

Proof (continued). Since $\psi_1, \psi_2 \in \mathcal{C}^1_{(2)}(\mathbb{R})$ then $\lim_{x\to\pm\infty} \psi_1(x) = \lim_{x\to\pm\infty} \psi_2(x) = \lim_{x\to\pm\infty} \frac{d\psi_1(x)}{dx} = \lim_{x\to\pm\infty} \frac{d\psi_2(x)}{dx} = 0$ and so

$$\lim_{a\to\infty} -\frac{\hbar^2}{2m}\left(\psi_1^* \frac{\psi_2}{dx} - \frac{d\psi_1^*}{dx}\psi_2\right)\Bigg|_{-a}^{a} = 0.$$

If we know $d^2\psi_1/dx^2, d^2\psi_2/dx^2 \in \mathcal{C}^1_{(2)}(\mathbb{R})$ then we know the inner product is defined and so the limit as $a \to \infty$ of the two integrals above exist, so that

$$\lim_{a\to\infty}\left(\int_{-a}^{a} \psi_1^*\left(-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2\right)dx\right)$$
$$= \lim_{a\to\infty}\left(\int_{-a}^{a}\left(-\frac{\hbar}{2m} d^2\psi_1^* dx^2 + V\psi_1^*\right)dx\right)$$

so the inner product claim of the theorem holds.

Theorem I.5.1 (continued 3)

Proof (continued). Since $\psi_1, \psi_2 \in \mathcal{C}^1_{(2)}(\mathbb{R})$ then $\lim_{x\to\pm\infty} \psi_1(x) = \lim_{x\to\pm\infty} \psi_2(x) = \lim_{x\to\pm\infty} \frac{d\psi_1(x)}{dx} = \lim_{x\to\pm\infty} \frac{d\psi_2(x)}{dx} = 0$ and so

$$\lim_{a\to\infty} -\frac{\hbar^2}{2m}\left(\psi_1^* \frac{\psi_2}{dx} - \frac{d\psi_1^*}{dx}\psi_2\right)\Bigg|_{-a}^{a} = 0.$$

If we know $d^2\psi_1/dx^2, d^2\psi_2/dx^2 \in \mathcal{C}^1_{(2)}(\mathbb{R})$ then we know the inner product is defined and so the limit as $a \to \infty$ of the two integrals above exist, so that

$$\lim_{a\to\infty}\left(\int_{-a}^{a} \psi_1^*\left(-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2\right)dx\right)$$

$$= \lim_{a\to\infty}\left(\int_{-a}^{a}\left(-\frac{\hbar}{2m}d^2\psi_1^* dx^2 + V\psi_1^*\right)dx\right)$$

so the inner product claim of the theorem holds. (BUT it does seem that we need the added assumption $d^2\psi_1/dx^2, d^2\psi_2/dx^2 \in \mathcal{C}^1_{(2)}(\mathbb{R})$ in order to insure convergence of the above integrals.

Theorem I.5.1 (continued 3)

Proof (continued). Since $\psi_1, \psi_2 \in \mathcal{C}^1_{(2)}(\mathbb{R})$ then $\lim_{x\to\pm\infty} \psi_1(x) = \lim_{x\to\pm\infty} \psi_2(x) = \lim_{x\to\pm\infty} \frac{d\psi_1(x)}{dx} = \lim_{x\to\pm\infty} \frac{d\psi_2(x)}{dx} = 0$ and so

$$\lim_{a\to\infty} -\frac{\hbar^2}{2m}\left(\psi_1^* \frac{\psi_2}{dx} - \frac{d\psi_1^*}{dx}\psi_2\right)\Bigg|_{-a}^{a} = 0.$$

If we know $d^2\psi_1/dx^2, d^2\psi_2/dx^2 \in \mathcal{C}^1_{(2)}(\mathbb{R})$ then we know the inner product is defined and so the limit as $a \to \infty$ of the two integrals above exist, so that

$$\lim_{a\to\infty}\left(\int_{-a}^{a} \psi_1^* \left(-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2\right)\, dx\right)$$
$$= \lim_{a\to\infty}\left(\int_{-a}^{a} \left(-\frac{\hbar}{2m} d^2\psi_1^* dx^2 + V\psi_1^*\right)\, dx\right)$$

so the inner product claim of the theorem holds. (BUT it does seem that we need the added assumption $d^2\psi_1/dx^2, d^2\psi_2/dx^2 \in \mathcal{C}^1_{(2)}(\mathbb{R})$ in order to insure convergence of the above integrals.

Theorem I.5.1 (continued 4)

Proof (continued). If we know that ψ_1 and ψ_2 satisfy the time-independent Schroedinger equation then we know $-\frac{\hbar^2}{2m}\frac{d^2\psi_i}{dx^2} = E_i\psi_i - V\psi_i \in \mathcal{C}^1_{(2)}(\mathbb{R})$ for $i = 1, 2$.)

If $\psi_1(x)$ and $\psi_2(x)$ satisfy the conditions of the theorem and if in addition they are solutions of the time-independent Schroedinger equation with eigenvalues E_1 and E_2 (so that the issue raised about $d^2\psi_1/dx^2$ and $d^2\psi_2/dx^2$ are not a concern) then by the first part of the theorem concerning inner products and from the time-independent Schroedinger equation we conclude $\langle \psi_1(x) \mid E_2\psi_2(x)\rangle = \langle E_1\psi_1(x) \mid \psi_2(x)\rangle$.

Theorem I.5.1 (continued 4)

Proof (continued). If we know that ψ_1 and ψ_2 satisfy the time-independent Schroedinger equation then we know $-\frac{\hbar^2}{2m}\frac{d^2\psi_i}{dx^2} = E_i\psi_i - V\psi_i \in \mathcal{C}^1_{(2)}(\mathbb{R})$ for $i = 1, 2$.)

If $\psi_1(x)$ and $\psi_2(x)$ satisfy the conditions of the theorem and if in addition they are solutions of the time-independent Schroedinger equation with eigenvalues E_1 and E_2 (so that the issue raised about $d^2\psi_1/dx^2$ and $d^2\psi_2/dx^2$ are not a concern) then by the first part of the theorem concerning inner products and from the time-independent Schroedinger equation we conclude $\langle \psi_1(x) \mid E_2\psi_2(x)\rangle = \langle E_1\psi_1(x) \mid \psi_2(x)\rangle$. If we take $\psi_1(x) = \psi_2(x) = \psi(x)$ and $E_1 = E_2 = E$ in this equation, then we get $E\langle \psi \mid \psi\rangle = \langle \psi \mid E\psi\rangle = \langle E\psi \mid \psi\rangle = E^*\langle \psi \mid \psi\rangle$. So if ψ is a nontrivial solution of the time-independent Schroedinger equation (i.e., $\psi(x) \not\equiv 0$) then $\|\psi\|^2 = \langle \psi \mid \psi\rangle > 0$ and so $E = E^*$ in this case. That is, the eigenvalues of the time-independent Schroedinger equation are real.

Theorem I.5.1 (continued 4)

Proof (continued). If we know that ψ_1 and ψ_2 satisfy the time-independent Schroedinger equation then we know $-\frac{\hbar^2}{2m}\frac{d^2\psi_i}{dx^2} = E_i\psi_i - V\psi_i \in \mathcal{C}^1_{(2)}(\mathbb{R})$ for $i = 1, 2$.)

If $\psi_1(x)$ and $\psi_2(x)$ satisfy the conditions of the theorem and if in addition they are solutions of the time-independent Schroedinger equation with eigenvalues E_1 and E_2 (so that the issue raised about $d^2\psi_1/dx^2$ and $d^2\psi_2/dx^2$ are not a concern) then by the first part of the theorem concerning inner products and from the time-independent Schroedinger equation we conclude $\langle \psi_1(x) \mid E_2\psi_2(x)\rangle = \langle E_1\psi_1(x) \mid \psi_2(x)\rangle$. If we take $\psi_1(x) = \psi_2(x) = \psi(x)$ and $E_1 = E_2 = E$ in this equation, then we get $E\langle \psi \mid \psi\rangle = \langle \psi \mid E\psi\rangle = \langle E\psi \mid \psi\rangle = E^*\langle \psi \mid \psi\rangle$. So if ψ is a nontrivial solution of the time-independent Schroedinger equation (i.e., $\psi(x) \not\equiv 0$) then $\|\psi\|^2 = \langle \psi \mid \psi\rangle > 0$ and so $E = E^*$ in this case. That is, the eigenvalues of the time-independent Schroedinger equation are real.

Theorem I.5.1 (continued 5)

Proof (continued). Finally, let ψ_1 and ψ_2 be solutions to the time-independent Schroedinger equation with associated eigenvalues E_1 and E_2, respectively, where $E_1 \neq E_2$. Then $\langle \psi_1 \mid E_2\psi_2 \rangle = \langle E_1\psi_1 \mid \psi_2 \rangle$, or (since E_1 and E_2 are real) $E_2\langle \psi_1 \mid \psi_2 \rangle = E_1\langle \psi_1 \mid \psi_2 \rangle$, or $(E_2 - E_1)\langle \psi_1 \mid \psi_2 \rangle = 0$. Since $E_1 \neq E_2$ then we must have $\psi_1 \perp \psi_2$, as claimed. $\square$

Theorem I.5.B

Theorem I.5.B. Let $\mathcal{H}_{\text{b}}^{(1)}$ be the (topologically) closed subspace of $\mathcal{H}^{(1)}$ which is spanned by $\mathcal{E}_{\text{b}}$ (where $\mathcal{E}_{\text{b}}$ is the set of "bound states"; that is, the set of $\mathcal{C}^1_{(2)}(\mathbb{R})$ which are solutions of the time-independent Schroedinger equations). Then an orthonormal basis of $\mathcal{H}_{\text{b}}^{(1)}$ is given by $T = \cup_{E \in S_{\text{p}}} T_E$ where T_E is an orthonormal basis for M_E. NOTE: You may assume that $\mathcal{H}^{(1)}$ is separable (as will be shown in Chapter II).

Proof. First, since we assume $\mathcal{H}^{(1)}$ is separable, then by Theorem I.4.2 $\mathcal{H}_{\text{b}}^{(1)}$ is also separable. For each $E \in S_{\text{b}}$, M_E is a subspace of $\mathcal{H}_{\text{b}}^{(1)}$ and so M_E is also separable. By Theorem I.4.5, each M_E has an at most countably infinite orthonormal system T_E spanning M_E.

Theorem I.5.B

Theorem I.5.B. Let $\mathcal{H}_{\mathrm{b}}^{(1)}$ be the (topologically) closed subspace of $\mathcal{H}^{(1)}$ which is spanned by $\mathcal{E}_{\mathrm{b}}$ (where $\mathcal{E}_{\mathrm{b}}$ is the set of "bound states"; that is, the set of $\mathcal{C}^1_{(2)}(\mathbb{R})$ which are solutions of the time-independent Schroedinger equations). Then an orthonormal basis of $\mathcal{H}_{\mathrm{b}}^{(1)}$ is given by $T = \cup_{E \in S_{\mathrm{p}}} T_E$ where T_E is an orthonormal basis for M_E. NOTE: You may assume that $\mathcal{H}^{(1)}$ is separable (as will be shown in Chapter II).

Proof. First, since we assume $\mathcal{H}^{(1)}$ is separable, then by Theorem I.4.2 $\mathcal{H}_{\mathrm{b}}^{(1)}$ is also separable. For each $E \in S_{\mathrm{b}}$, M_E is a subspace of $\mathcal{H}_{\mathrm{b}}^{(1)}$ and so M_E is also separable. By Theorem I.4.5, each M_E has an at most countably infinite orthonormal system T_E spanning M_E. Consider $T = \cup_{E \in S_{\mathrm{p}}} T_E$. Now every element of $\mathcal{E}_{\mathrm{b}}$ is some (countable) sum of elements of T. Since the closure of the span of $\mathcal{E}_{\mathrm{b}}$ is $\mathcal{H}_{\mathrm{b}}^{(1)}$, then the closed subspace spanned by T is $\mathcal{H}_{\mathrm{b}}^{(1)}$.

Theorem I.5.B

Theorem I.5.B. Let $\mathcal{H}_{\text{b}}^{(1)}$ be the (topologically) closed subspace of $\mathcal{H}^{(1)}$ which is spanned by $\mathcal{E}_{\text{b}}$ (where $\mathcal{E}_{\text{b}}$ is the set of "bound states"; that is, the set of $\mathcal{C}^1_{(2)}(\mathbb{R})$ which are solutions of the time-independent Schroedinger equations). Then an orthonormal basis of $\mathcal{H}_{\text{b}}^{(1)}$ is given by $T = \cup_{E \in S_{\text{p}}} T_E$ where T_E is an orthonormal basis for M_E. NOTE: You may assume that $\mathcal{H}^{(1)}$ is separable (as will be shown in Chapter II).

Proof. First, since we assume $\mathcal{H}^{(1)}$ is separable, then by Theorem I.4.2 $\mathcal{H}_{\text{b}}^{(1)}$ is also separable. For each $E \in S_{\text{b}}$, M_E is a subspace of $\mathcal{H}_{\text{b}}^{(1)}$ and so M_E is also separable. By Theorem I.4.5, each M_E has an at most countably infinite orthonormal system T_E spanning M_E. Consider $T = \cup_{E \in S_{\text{p}}} T_E$. Now every element of $\mathcal{E}_{\text{b}}$ is some (countable) sum of elements of T. Since the closure of the span of $\mathcal{E}_{\text{b}}$ is $\mathcal{H}_{\text{b}}^{(1)}$, then the closed subspace spanned by T is $\mathcal{H}_{\text{b}}^{(1)}$.

Theorem I.5.B (continued)

Theorem I.5.B. Let $\mathcal{H}_{\mathrm{b}}^{(1)}$ be the (topologically) closed subspace of $\mathcal{H}^{(1)}$ which is spanned by $\mathcal{E}_{\mathrm{b}}$ (where $\mathcal{E}_{\mathrm{b}}$ is the set of "bound states"; that is, the set of $\mathcal{C}^1_{(2)}(\mathbb{R})$ which are solutions of the time-independent Schroedinger equations). Then an orthonormal basis of $\mathcal{H}_{\mathrm{b}}^{(1)}$ is given by $T = \cup_{E \in S_{\mathrm{p}}} T_E$ where T_E is an orthonormal basis for M_E. NOTE: You may assume that $\mathcal{H}^{(1)}$ is separable (as will be shown in Chapter II).

Proof (continued). Since each T_E is orthonormal and by Theorem I.5.1 every element of T_{E_1} is orthonormal to every subset of T_{E_2} for $E_1 \neq E_2$, then set T is orthonormal. So T is linearly independent (see Exercise I.4.12) and by Exercise I.5.3, T is countable. So T is an orthonormal basis of $\mathcal{H}_{\mathrm{b}}^{(1)}$, as claimed. □

Theorem I.5.2

Theorem I.5.2. For any fixed $t \in \mathbb{R}$, the sequence $\{\Phi_1(t), \Phi_2(t), \ldots\}$,

$$\Phi_n(t) = \sum_{k=1}^{n} c_k(t)\Psi_k$$

$$\text{where } c_k(t) = \exp\left(-\frac{i}{\hbar}E_k(t - t_0)\right)\langle \Psi_k \mid \Psi_0 \rangle,$$

is convergent in the norm of $\mathcal{H}_{\mathrm{b}}^{(1)}$ to some $\Psi(t) \in \mathcal{H}_{\mathrm{b}}^{(1)}$. For $t = t_0$, $\lim_{n\to\infty} \Phi_n(t_0) = \Psi(t_0)$ satisfies the initial condition $\Psi(t_0) = \Psi_0$.

Proof. Since $\{\Psi_1, \Psi_2, \ldots\}$ is an orthonormal basis in $\mathcal{H}_{\mathrm{b}}^{(1)}$, by Theorem I.4.6(d),

$$\sum_{k=1}^{\infty} |c_k(t)|^2 = \sum_{k=1}^{\infty} \left| \exp\left(-\frac{i}{\hbar}E_k(t - t_0)\right)\langle \Psi_k \mid \Psi_0 \rangle \right|^2$$

Theorem I.5.2

Theorem I.5.2. For any fixed $t \in \mathbb{R}$, the sequence $\{\Phi_1(t), \Phi_2(t), \ldots\}$,

$$\Phi_n(t) = \sum_{k=1}^{n} c_k(t)\Psi_k$$

$$\text{where } c_k(t) = \exp\left(-\frac{i}{\hbar}E_k(t - t_0)\right)\langle \Psi_k \mid \Psi_0 \rangle,$$

is convergent in the norm of $\mathcal{H}_{\mathrm{b}}^{(1)}$ to some $\Psi(t) \in \mathcal{H}_{\mathrm{b}}^{(1)}$. For $t = t_0$, $\lim_{n\to\infty} \Phi_n(t_0) = \Psi(t_0)$ satisfies the initial condition $\Psi(t_0) = \Psi_0$.

Proof. Since $\{\Psi_1, \Psi_2, \ldots\}$ is an orthonormal basis in $\mathcal{H}_{\mathrm{b}}^{(1)}$, by Theorem I.4.6(d),

$$\sum_{k=1}^{\infty} |c_k(t)|^2 = \sum_{k=1}^{\infty} \left| \exp\left(-\frac{i}{\hbar}E_k(t - t_0)\right)\langle \Psi_k \mid \Psi_0 \rangle \right|^2$$

Theorem I.5.2 (continued 1)

Proof (continued).

$$\begin{aligned}\sum_{k=1}^{\infty}|c_k(t)|^2 &= \sum_{k=1}^{\infty}|\langle\Psi_k \mid \Psi_0\rangle|^2 \text{ since } \left|\exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\right| = 1 \\ &\quad \text{because } E_k \text{ is real by Theorem I.5.1} \\ &= \|\Psi_0\|^2 < \infty.\end{aligned}$$

So for given $\varepsilon > 0$, there is $N \in \mathbb{N}$ such that $\sum_{k=N}^{\infty}|c_k(t)|^2 < \varepsilon^2$. So if $m, n > N$ (with $m \geq n$, say) then

$$|\Phi_m(t) - \Phi_n(t)|^2 = \left|\sum_{k=n}^{m} c_k(t)\Psi_k\right|^2 = \sum_{k=n}^{m}|c_k(t)|^2 \leq \sum_{k=N}^{\infty}|c_k(t)|^2 < \varepsilon^2,$$

and so $\{\Phi_n(t)\}$ is a Cauchy sequence in $\mathcal{H}_{\mathrm{b}}^{(1)}$ and hence, since $\mathcal{H}_{\mathrm{b}}^{(1)}$ is complete, converges to some $\Psi(t) \in \mathcal{H}_{\mathrm{b}}^{(1)}$.

Theorem I.5.2 (continued 1)

Proof (continued).

$$\begin{aligned}\sum_{k=1}^{\infty}|c_k(t)|^2 &= \sum_{k=1}^{\infty}|\langle\Psi_k \mid \Psi_0\rangle|^2 \text{ since } \left|\exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\right| = 1\\ &\quad\text{because } E_k \text{ is real by Theorem I.5.1}\\ &= \|\Psi_0\|^2 < \infty.\end{aligned}$$

So for given $\varepsilon > 0$, there is $N \in \mathbb{N}$ such that $\sum_{k=N}^{\infty}|c_k(t)|^2 < \varepsilon^2$. So if $m, n > N$ (with $m \geq n$, say) then

$$|\Phi_m(t) - \Phi_n(t)|^2 = \left|\sum_{k=n}^{m} c_k(t)\Psi_k\right|^2 = \sum_{k=n}^{m}|c_k(t)|^2 \leq \sum_{k=N}^{\infty}|c_k(t)|^2 < \varepsilon^2,$$

and so $\{\Phi_n(t)\}$ is a Cauchy sequence in $\mathcal{H}_{\mathrm{b}}^{(1)}$ and hence, since $\mathcal{H}_{\mathrm{b}}^{(1)}$ is complete, converges to some $\Psi(t) \in \mathcal{H}_{\mathrm{b}}^{(1)}$.

Theorem I.5.2 (continued 2)

Theorem I.5.2. For any fixed $t \in \mathbb{R}$, the sequence $\{\Phi_1(t), \Phi_2(t), \ldots\}$,

$$\Phi_n(t) = \sum_{k=1}^{n} c_k(t)\Psi_k$$
$$\text{where } c_k(t) = \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle\Psi_k \mid \Psi_0\rangle,$$

is convergent in the norm of $\mathcal{H}_{\mathrm{b}}^{(1)}$ to some $\Psi(t) \in \mathcal{H}_{\mathrm{b}}^{(1)}$. For $t = t_0$, $\lim_{n\to\infty} \Phi_n(t_0) = \Psi(t_0)$ satisfies the initial condition $\Psi(t_0) = \Psi_0$.

Proof (continued). With $t = t_0$, $c_k = \langle\Psi_k \mid \Psi_0\rangle$ for $k \in \mathbb{N}$ and so

$$\Psi(t_0) = \lim_{n\to\infty} \Phi_n(t_0) = \lim_{n\to\infty} \sum_{k=1}^{n} c_k(t_0)\Psi_k = \sum_{k=1}^{\infty} c_k(t_0)\Psi_k = \sum_{k=1}^{\infty} \langle\Psi_k \mid \Psi_0\rangle\Psi_k$$

by Theorem I.4.6, as claimed. □

Theorem I.5.C

Theorem I.5.C. Suppose the series

$$\sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar} E_k(t - t_0)\right) \langle \Psi_k \mid \Psi_0 \rangle \varphi_k(x)$$

converges in the $\mathcal{H}_{\mathrm{b}}^{(1)}$ norm for each fixed value of t and converges pointwise for each value of x and t to a limit function $\varphi(x, t)$, and that $\partial^2\varphi(x, t)/\partial x^2$ and $\partial\psi(x, t)/\partial t$ can be obtained by differentiating the series term by term twice in x and once in t. Here, $\varphi_k(x)$ satisfies the time-independent Schroedinger equation for $E = E_k$. Then $\varphi(x, t)$ is a solution to Schroedinger's equation

$$i\hbar \frac{\partial \varphi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \varphi(x, t)}{\partial x^2} + V(x)\varphi(x, t).$$

Theorem I.5.C (continued)

Proof. By the hypotheses on differentiability, we have

$$\begin{aligned} \frac{\partial \varphi(x,t)}{\partial t} &= -\frac{i}{\hbar}\sum_{k=1}^{\infty} E_k \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle \frac{d\varphi_k(x)}{dt} \\ \frac{\partial^2 \varphi(x,t)}{\partial x^2} &= \sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle \frac{d^2\varphi_k(x)}{dx^2} \end{aligned}$$

(notice the inner product is an integral over x so $\langle \Psi_k \mid \Psi_0\rangle$ is a constant). So

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x,t)}{\partial x^2} + V(x)\varphi(x,t)$$

$$= -\frac{\hbar}{2m}\sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle \frac{d^2\varphi_k(x)}{dx^2}$$

$$V(x)\sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle \varphi_k(x)$$

Theorem I.5.C (continued)

Proof. By the hypotheses on differentiability, we have

$$\begin{aligned}
\frac{\partial \varphi(x,t)}{\partial t} &= -\frac{i}{\hbar}\sum_{k=1}^{\infty} E_k \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle \frac{d\varphi_k(x)}{dt} \\
\frac{\partial^2 \varphi(x,t)}{\partial x^2} &= \sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle \frac{d^2\varphi_k(x)}{dx^2}
\end{aligned}$$

(notice the inner product is an integral over x so $\langle \Psi_k \mid \Psi_0\rangle$ is a constant). So

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi(x,t)}{\partial x^2} + V(x)\varphi(x,t)$$

$$\begin{aligned}
= \quad & -\frac{\hbar}{2m}\sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle \frac{d^2\varphi_k(x)}{dx^2} \\
& V(x)\sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle \varphi_k(x)
\end{aligned}$$

Theorem I.5.C (continued)

Proof (continued).

$$= \sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle\Psi_k \mid \Psi_0\rangle\left(-\frac{\hbar^2}{2m}\frac{d^2\varphi_k(x)}{dx^2}+V(x)\varphi_k(x)\right)$$

$$= \sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle\Psi_k \mid \Psi_0\rangle E_k\varphi_k(x)$$

since $\varphi_k(x)$ is a solution to the time-independent Schroedinger equation for $E = E_k : -\frac{\hbar^2}{2m}\frac{d^2\varphi_k(x)}{dx^2}+V(x)\varphi_k(x) = E_k\varphi_k(x)$

$$= \frac{\hbar}{-i}\frac{\partial\varphi(x,t)}{\partial t} = i\hbar\frac{\partial\varphi(x,t)}{\partial t}.$$

So

$$\varphi(x,t) = \sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle\Psi_k \mid \Psi_0\rangle\varphi_k(x)$$

is a solution to the Schroedinger equation, as claimed. □

Theorem I.5.C (continued)

Proof (continued).

$$= \sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle \left(-\frac{\hbar^2}{2m}\frac{d^2\varphi_k(x)}{dx^2} + V(x)\varphi_k(x)\right)$$

$$= \sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle E_k\varphi_k(x)$$

since $\varphi_k(x)$ is a solution to the time-independent Schroedinger equation for $E = E_k$: $-\frac{\hbar^2}{2m}\frac{d^2\varphi_k(x)}{dx^2} + V(x)\varphi_k(x) = E_k\varphi_k(x)$

$$= \frac{\hbar}{-i}\frac{\partial\varphi(x,t)}{\partial t} = i\hbar\frac{\partial\varphi(x,t)}{\partial t}.$$

So

$$\varphi(x,t) = \sum_{k=1}^{\infty} \exp\left(-\frac{i}{\hbar}E_k(t-t_0)\right)\langle \Psi_k \mid \Psi_0\rangle\varphi_k(x)$$

is a solution to the Schroedinger equation, as claimed. □

Theorem I.5.D

Theorem I.5.D. The general solution of

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0 \text{ for } 0 \le x \le L$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi(x) = 0 \text{ for } x < 0, x > L$$

is

$$\psi(x) = \begin{cases} ce^{ikx} + de^{-ikx} \text{ where } k = \sqrt{2mE}/\hbar \text{ for } 0 \le x \le L \\ a_1 e^{-ik'x} + b_1 e^{ik'x} \text{ where } k' = \sqrt{2m(E - V_0)}/\hbar \text{ for } x < 0 \\ a_2 e^{ik''x} + b_2 e^{-ik''x} \text{ where } k'' = \sqrt{2m(E - V_0)}/\hbar \text{ for } x > L. \end{cases}$$

Proof. Since the ODE is second order linear and in each of the three regions $\psi(x)$ is a linear combination of two linearly independent functions, we just need to confirm that $\psi(x)$ satisfies the ODE in each region.

Theorem I.5.D

Theorem I.5.D. The general solution of

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0 \text{ for } 0 \le x \le L$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi(x) = 0 \text{ for } x < 0, x > L$$

is

$$\psi(x) = \begin{cases} ce^{ikx} + de^{-ikx} \text{ where } k = \sqrt{2mE}/\hbar \text{ for } 0 \le x \le L \\ a_1 e^{-ik'x} + b_1 e^{ik'x} \text{ where } k' = \sqrt{2m(E - V_0)}/\hbar \text{ for } x < 0 \\ a_2 e^{ik''x} + b_2 e^{-ik''x} \text{ where } k'' = \sqrt{2m(E - V_0)}/\hbar \text{ for } x > L. \end{cases}$$

Proof. Since the ODE is second order linear and in each of the three regions $\psi(x)$ is a linear combination of two linearly independent functions, we just need to confirm that $\psi(x)$ satisfies the ODE in each region.

Theorem I.5.D (continued)

Proof (continued). For $0 \leq x \leq L$ we have

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = -k^2ce^{ikx} - k^2de^{-kx} + \frac{2m}{\hbar^2}E(ce^{ikx} + de^{-ikx})$$
$$= -\frac{2mE}{\hbar^2}ce^{ikx} - \frac{2mE}{\hbar^2}de^{-ikx} + \frac{2m}{\hbar^2}Ece^{ikx} + \frac{2m}{\hbar^2}de^{-ikx} = 0.$$

For $x < 0$ (and similarly for $x > L$),

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = -(k')^2a_1e^{-ik'x} - (k')^2b_1e^{-k'x}$$
$$+\frac{2m}{\hbar^2}(E - V_0)(a_1e^{-ik'x} + b_1e^{ik'x})$$
$$= -\frac{2m(E - V_0)}{\hbar^2}a_1e^{-ik'x} - \frac{2m(E - V_0)}{\hbar^2}b_1e^{-k'x}$$
$$+\frac{2m(E - V_0)}{\hbar^2}a_1e^{-ik'x} + \frac{2m(E - V_0)}{\hbar^2}b_1e^{ik'x} = 0.$$

□

Theorem I.5.D (continued)

Proof (continued). For $0 \le x \le L$ we have

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = -k^2ce^{ikx} - k^2de^{-kx} + \frac{2m}{\hbar^2}E(ce^{ikx} + de^{-ikx})$$
$$= -\frac{2mE}{\hbar^2}ce^{ikx} - \frac{2mE}{\hbar^2}de^{-ikx} + \frac{2m}{\hbar^2}Ece^{ikx} + \frac{2m}{\hbar^2}de^{-ikx} = 0.$$

For $x < 0$ (and similarly for $x > L$),

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = -(k')^2a_1e^{-ik'x} - (k')^2b_1e^{-k'x}$$
$$+\frac{2m}{\hbar^2}(E - V_0)(a_1e^{-ik'x} + b_1e^{ik'x})$$
$$= -\frac{2m(E - V_0)}{\hbar^2}a_1e^{-ik'x} - \frac{2m(E - V_0)}{\hbar^2}b_1e^{-k'x}$$
$$+\frac{2m(E - V_0)}{\hbar^2}a_1e^{-ik'x} + \frac{2m(E - V_0)}{\hbar^2}b_1e^{ik'x} = 0.$$

□