A Course in Mechanics by Dr. J. Tinsley Oden
Part II - Homework 3 - Solutions

Pablo Seleson

November 30, 2010

Set II.2:

7. In this exercise, we use time-independent wave functions for simplicity.

   (a) We check whether e^{ix} is Hermitian:

$$\langle \psi(x), e^{ix}\phi(x)\rangle = \int_{-\infty}^{\infty} \psi^*(x)e^{ix}\phi(x)dx,$$
$$\langle e^{ix}\psi(x), \phi(x)\rangle = \int_{-\infty}^{\infty} e^{-ix}\psi^*(x)\phi(x)dx = \int_{-\infty}^{\infty} \psi^*(x)e^{-ix}\phi(x)dx \neq \langle \psi(x), e^{ix}\phi(x)\rangle.$$

   Then, the operator is not Hermitian.

   (b) We check whether $\frac{d^2}{dx^2}$ is Hermitian:

$$\langle \psi(x), \frac{d^2}{dx^2}\phi(x)\rangle = \int_{-\infty}^{\infty} \psi^*(x)\frac{d^2\phi}{dx^2}(x)dx = \psi^*(x)\frac{d\phi}{dx}(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\psi^*}{dx}(x)\frac{d\phi}{dx}(x)dx$$
$$= -\int_{-\infty}^{\infty} \frac{d\psi^*}{dx}(x)\frac{d\phi}{dx}(x)dx,$$

   where we used integration by parts, and the fact that $\psi(x) \to 0$ for $x \to \pm\infty$ and we assume the wave function derivatives are bounded. By another integration by parts we obtain

$$\langle \psi(x), \frac{d^2}{dx^2}\phi(x)\rangle = -\frac{d\psi^*}{dx}(x)\phi(x)\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{d^2\psi^*}{dx^2}(x)\phi(x)dx = \int_{-\infty}^{\infty} \frac{d^2\psi^*}{dx^2}(x)\phi(x)dx,$$

   where the boundary terms vanish as before. Therefore,

$$\boxed{\langle \psi(x), \frac{d^2}{dx^2}\phi(x)\rangle = \langle \frac{d^2}{dx^2}\psi(x), \phi(x)\rangle},$$

   and thus the operator is Hermitian.

(c) We check whether $x\frac{d}{dx}$ is Hermitian:

$$\begin{aligned}
\langle \psi(x), x\frac{d}{dx}\phi(x)\rangle &= \int_{-\infty}^{\infty} \psi^*(x)x\frac{d\phi}{dx}(x)dx \\
&= \psi^*(x)x\phi(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{d\psi^*}{dx}(x)x\phi(x)dx - \int_{-\infty}^{\infty}\psi^*(x)\phi(x)dx \\
&= -\langle x\frac{d}{dx}\psi(x), \phi(x)\rangle - \langle \psi(x), \phi(x)\rangle \neq \langle x\frac{d}{dx}\psi(x), \phi(x)\rangle,
\end{aligned}$$

where we used integration by parts and assumed wave functions decay fast enough so that $\sqrt{x}\phi(x) \to= 0$ and $\sqrt{x}\psi^*(x) \to= 0$ as $x \to \pm\infty$. This assumption implies $\langle x\rangle$ is bounded. Thus, the operator is not Hermitian.

8. a)

$$\begin{aligned}
\frac{\mathrm{d}\langle Q\rangle}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\langle \Psi(x,t), \tilde{Q}\Psi(x,t)\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^3}\Psi^*(x,t)\tilde{Q}\Psi(x,t)d^3x \\
&= \int_{\mathbb{R}^3}\frac{\partial\Psi^*}{\partial t}(x,t)\tilde{Q}\Psi(x,t)d^3x + \int_{\mathbb{R}^3}\Psi^*(x,t)\frac{\partial\tilde{Q}}{\partial t}\Psi(x,t)d^3x + \int_{\mathbb{R}^3}\Psi^*(x,t)\tilde{Q}\frac{\partial\Psi}{\partial t}(x,t)d^3x \\
&= \int_{\mathbb{R}^3}\frac{\partial\Psi^*}{\partial t}(x,t)\tilde{Q}\Psi(x,t)d^3x + \left\langle\frac{\partial\tilde{Q}}{\partial t}\right\rangle + \int_{\mathbb{R}^3}\Psi^*(x,t)\tilde{Q}\frac{\partial\Psi}{\partial t}(x,t)d^3x.
\end{aligned}$$

b) Following Schrödinger's equation

$$\begin{aligned}
\frac{\partial\Psi}{\partial t} &= \frac{1}{i\hbar}H\Psi = \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\Delta + V\right)\Psi, \\
\Rightarrow \frac{\partial\Psi^*}{\partial t} &= -\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\Delta + V\right)\Psi^* = -\frac{1}{i\hbar}H\Psi^*.
\end{aligned}$$

c) Using the Hermitian property of H we proceed as follows

$$\begin{aligned}
\frac{\mathrm{d}\langle Q\rangle}{\mathrm{d}t} &= \int_{\mathbb{R}^3} -\frac{1}{i\hbar}H\Psi^*(x,t)\tilde{Q}\Psi(x,t)d^3x + \left\langle\frac{\partial\tilde{Q}}{\partial t}\right\rangle + \int_{\mathbb{R}^3}\Psi^*(x,t)\tilde{Q}\frac{1}{i\hbar}H\Psi(x,t)d^3x \\
&= -\frac{1}{i\hbar}\int_{\mathbb{R}^3}\Psi^*(x,t)H\tilde{Q}\Psi(x,t)d^3x + \left\langle\frac{\partial\tilde{Q}}{\partial t}\right\rangle + \frac{1}{i\hbar}\int_{\mathbb{R}^3}\Psi^*(x,t)\tilde{Q}H\Psi(x,t)d^3x \\
&= \frac{1}{i\hbar}\int_{\mathbb{R}^3}\Psi^*(x,t)\left(\tilde{Q}H - H\tilde{Q}\right)\Psi(x,t)d^3x + \left\langle\frac{\partial\tilde{Q}}{\partial t}\right\rangle \\
&= \frac{1}{i\hbar}\int_{\mathbb{R}^3}\Psi^*(x,t)\left[\tilde{Q},H\right]\Psi(x,t)d^3x + \left\langle\frac{\partial\tilde{Q}}{\partial t}\right\rangle = \frac{1}{i\hbar}\left\langle\left[\tilde{Q},H\right]\right\rangle + \left\langle\frac{\partial\tilde{Q}}{\partial t}\right\rangle,
\end{aligned}$$

then we have

$$\boxed{\frac{\mathrm{d}\langle Q\rangle}{\mathrm{d}t} = \frac{1}{i\hbar}\left\langle\left[\tilde{Q},H\right]\right\rangle + \left\langle\frac{\partial\tilde{Q}}{\partial t}\right\rangle}.$$

Set II.3:

1. a) Considering the time-independent Schrödinger's equation

$$\begin{aligned} -\frac{\hbar^2}{2m}\Delta\psi(x,y) &= E\psi(x,y) && \text{in } \overline{\Omega}, \\ \psi(x,y) &= 0 && \text{on } \partial\overline{\Omega}. \end{aligned}$$

We find a solution using the method of separation of variables: $\psi(x,y) = X(x)Y(y)$. Then, the equation in $\overline{\Omega}$ is

$$\begin{aligned} -\frac{\hbar^2}{2m}\Delta\psi(x,y) &= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)X(x)Y(y) = -\frac{\hbar^2}{2m}\left(Y(y)\frac{d^2X}{dx^2}(x) + X(x)\frac{d^2Y}{dy^2}(y)\right) \\ &= EX(x)Y(y), \end{aligned}$$

or dividing by $X(x)Y(y)$ (assuming $X(x)Y(y) \neq 0$)

$$\left(-\frac{\hbar^2}{2m}\frac{1}{X(x)}\frac{d^2X}{dx^2}(x)\right) + \left(-\frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{d^2Y}{dy^2}(y)\right) = E.$$

Because each term depends on a different variable, a solution exists if each term is a constant and the sum of those constants equals E. Denote the constants e_X and e_Y, then

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2X}{dx^2}(x) &= e_X X(x), \quad x \in (0,a) \\ -\frac{\hbar^2}{2m}\frac{d^2Y}{dy^2}(y) &= e_Y Y(y), \quad y \in (0,b), \end{aligned}$$

with $e_X + e_Y = E$. The general solutions (assuming e_X and e_Y are positive) are

$$\begin{aligned} X(x) &= A\sin(k_x x) + B\cos(k_x x), \\ Y(y) &= C\sin(k_y y) + D\cos(k_y y), \end{aligned}$$

where

$$\frac{\hbar^2}{2m}k_x^2 = e_X, \quad \text{and} \quad \frac{\hbar^2}{2m}k_y^2 = e_Y.$$

Using the boundary conditions, we get

$$\begin{aligned} &X(0) = 0 \Rightarrow B = 0, \\ &X(a) = 0 = A\sin(k_x a) \Rightarrow k_x a = n\pi, \\ &Y(0) = 0 \Rightarrow D = 0, \\ &Y(b) = 0 = C\sin(k_y b) \Rightarrow k_y b = n'\pi, \end{aligned}$$

with n, n', nonzero integers. We now use the normalization to find A and C.

$$1 = \int_0^a |X(x)|^2 dx = A^2\int_0^a \sin^2(k_x x)dx = A^2\left(\frac{x}{2} - \frac{\sin(2k_x x)}{4k_x}\right)\Bigg|_0^a = A^2\frac{a}{2} \Rightarrow A = \pm\sqrt{\frac{2}{a}}.$$

Similarly,

$$1 = \int_0^b |Y(y)|^2 dy = C^2 \frac{b}{2} \Rightarrow C = \pm\sqrt{\frac{2}{b}}.$$

Then, choosing the positive normalizations, the solution is of the form

$$\boxed{\psi(x,y) = X(x)Y(y) = \sqrt{\frac{4}{ab}} \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{n'\pi}{b}y\right)}.$$

b) We now observe that

$$k_x^2 = \frac{2me_X}{\hbar^2} = \left(\frac{n\pi}{a}\right)^2 \Rightarrow e_X = \frac{n^2\hbar^2\pi^2}{2ma^2},$$
$$k_y^2 = \frac{2me_Y}{\hbar^2} = \left(\frac{n'\pi}{b}\right)^2 \Rightarrow e_Y = \frac{n'^2\hbar^2\pi^2}{2mb^2}.$$

The energy levels are $E = e_X + e_Y$, then

$$\boxed{E = \frac{\hbar^2\pi^2}{2m}\left(\frac{n^2}{a^2} + \frac{n'^2}{b^2}\right)}.$$

c) Assume a square box ($a = b$). Denote the energy levels by $\mu_{nn'}$, then

$$\mu_{nn'} = \frac{\hbar^2\pi^2}{2ma^2}\left(n^2 + n'^2\right),$$

for $n = 1, 2, \ldots$ and $n' = 1, 2, \ldots$. The lowest energy level occurs for $n = n' = 1$ and is

$$\boxed{\mu_{11} = \frac{\hbar^2\pi^2}{ma^2}}.$$

We then have

$$\mu_{nn'} = \left(\frac{n^2 + n'^2}{2}\right)\mu_{11}.$$

The following levels corresponding to n and n' up to 4 are:

$$\begin{aligned}
\mu_{12} = \mu_{21} &= \frac{5}{2}\mu_{11}, & \mu_{33} &= \frac{18}{2}\mu_{11},\\
\mu_{22} &= \frac{8}{2}\mu_{11}, & \mu_{24} = \mu_{42} &= \frac{20}{2}\mu_{11},\\
\mu_{13} = \mu_{31} &= \frac{10}{2}\mu_{11}, & \mu_{34} = \mu_{43} &= \frac{25}{2}\mu_{11},\\
\mu_{23} = \mu_{32} &= \frac{13}{2}\mu_{11}, & \mu_{44} &= \frac{32}{2}\mu_{11},\\
\mu_{14} = \mu_{41} &= \frac{17}{2}\mu_{11}.
\end{aligned}$$

<u>Note</u>: Notice that some states are degenerate.

2. a) Let $\mathbf{R} = \dfrac{\mathbf{r}_1 M + \mathbf{r}_2 m}{M+m}$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. Then,

$$M\mathbf{r}_1 = (M+m)\mathbf{R} - \mathbf{r}_2 m = (M+m)\mathbf{R} - (\mathbf{r}_1 - \mathbf{r})m$$
$$\mathbf{r}_1 = \mathbf{R} + \frac{m}{M+m}\mathbf{r} = \mathbf{R} + \frac{1}{M}\frac{Mm}{M+m}\mathbf{r}.$$

Furthermore,

$$m\mathbf{r}_2 = (M+m)\mathbf{R} - \mathbf{r}_1 M = (M+m)\mathbf{R} - (\mathbf{r} + \mathbf{r}_2)\, M,$$
$$\mathbf{r}_2 = \mathbf{R} - \frac{M}{M+m}\mathbf{r} = \mathbf{R} - \frac{1}{m}\frac{mM}{M+m}\mathbf{r}.$$

Let $m^* = \frac{mM}{M+m}$, then

$$\boxed{\mathbf{r}_1 = \mathbf{R} + \frac{m^*}{M}\mathbf{r}; \quad \mathbf{r}_2 = \mathbf{R} - \frac{m^*}{m}\mathbf{r}}.$$

b) Using the chain rule

$$\frac{\partial}{\partial(r_1)_i} = \frac{\partial}{\partial R_k}\frac{\partial R_k}{\partial(r_1)_i} + \frac{\partial}{\partial r_k}\frac{\partial r_k}{\partial(r_1)_i} = \frac{M}{M+m}\delta_{ki}\frac{\partial}{\partial R_k} + \delta_{ki}\frac{\partial}{\partial r_k} = \frac{m^*}{m}\frac{\partial}{\partial R_i} + \frac{\partial}{\partial r_i}.$$

Similarly,

$$\frac{\partial}{\partial(r_2)_i} = \frac{\partial}{\partial R_k}\frac{\partial R_k}{\partial(r_2)_i} + \frac{\partial}{\partial r_k}\frac{\partial r_k}{\partial(r_2)_i} = \frac{m}{M+m}\delta_{ki}\frac{\partial}{\partial R_k} - \delta_{ki}\frac{\partial}{\partial r_k} = \frac{m^*}{M}\frac{\partial}{\partial R_i} + \frac{\partial}{\partial r_i}.$$

Then, we have

$$\boxed{\nabla_{\mathbf{r}_1} = \frac{m^*}{m}\nabla_{\mathbf{R}} + \nabla_{\mathbf{r}}; \quad \nabla_{\mathbf{r}_2} = \frac{m^*}{M}\nabla_{\mathbf{R}} - \nabla_{\mathbf{r}}}.$$

c) The Schrödinger's equation for this two-particle system is

$$\left(-\frac{\hbar^2}{2M}\Delta_{\mathbf{r}_1} - \frac{\hbar^2}{2m}\Delta_{\mathbf{r}_2} + V(\mathbf{r})\right)\Psi(\mathbf{r}_1,\mathbf{r}_2,t) = i\hbar\frac{\partial\Psi}{\partial t}(\mathbf{r}_1,\mathbf{r}_2,t).$$

Assume a solution, using separation of variables, of the form $\Psi(\mathbf{r}_1,\mathbf{r}_2,t) = \psi(\mathbf{r}_1,\mathbf{r}_2)e^{-iEt/\hbar}$. Then, we get

$$\left(-\frac{\hbar^2}{2M}\Delta_{\mathbf{r}_1} - \frac{\hbar^2}{2m}\Delta_{\mathbf{r}_2} + V(\mathbf{r})\right)\psi(\mathbf{r}_1,\mathbf{r}_2)\cancel{e^{-iEt/\hbar}} = E\psi(\mathbf{r}_1,\mathbf{r}_2)\cancel{e^{-iEt/\hbar}}.$$

Thus, the time independent Schrödinger's equation is

$$\left(-\frac{\hbar^2}{2M}\Delta_{\mathbf{r}_1} - \frac{\hbar^2}{2m}\Delta_{\mathbf{r}_2} + V(\mathbf{r})\right)\psi(\mathbf{r}_1,\mathbf{r}_2) = E\psi(\mathbf{r}_1,\mathbf{r}_2).$$

We now want to write this expression using the variables $\mathbf{R}$ and $\mathbf{r}$. Then,

$$\Delta_{\mathbf{r}_1} = \nabla_{\mathbf{r}_1}\cdot\nabla_{\mathbf{r}_1} = \left(\frac{m^*}{m}\nabla_{\mathbf{R}} + \nabla_{\mathbf{r}}\right)\cdot\left(\frac{m^*}{m}\nabla_{\mathbf{R}} + \nabla_{\mathbf{r}}\right) = \left(\frac{m^*}{m}\right)^2\Delta_{\mathbf{R}} + 2\frac{m^*}{m}\nabla_{\mathbf{R}}\cdot\nabla_{\mathbf{r}} + \Delta_{\mathbf{r}},$$
$$\Delta_{\mathbf{r}_2} = \nabla_{\mathbf{r}_2}\cdot\nabla_{\mathbf{r}_2} = \left(\frac{m^*}{M}\nabla_{\mathbf{R}} - \nabla_{\mathbf{r}}\right)\cdot\left(\frac{m^*}{M}\nabla_{\mathbf{R}} - \nabla_{\mathbf{r}}\right) = \left(\frac{m^*}{M}\right)^2\Delta_{\mathbf{R}} - 2\frac{m^*}{M}\nabla_{\mathbf{R}}\cdot\nabla_{\mathbf{r}} + \Delta_{\mathbf{r}}.$$

$$
\begin{aligned}
-\frac{\hbar^2}{2M}\Delta_{\mathbf{r}_1} - \frac{\hbar^2}{2m}\Delta_{\mathbf{r}_2} &= -\frac{\hbar^2}{2M}\left(\frac{m^*}{m}\right)^2\Delta_{\mathbf{R}} - \frac{\hbar^2}{2M}\Delta_{\mathbf{r}} - \frac{\hbar^2}{2m}\left(\frac{m^*}{M}\right)^2\Delta_{\mathbf{R}} - \frac{\hbar^2}{2m}\Delta_{\mathbf{r}} \\
&= -\frac{\hbar^2}{2}\left(\frac{1}{M}\left(\frac{m^*}{m}\right)^2 + \frac{1}{m}\left(\frac{m^*}{M}\right)^2\right)\Delta_{\mathbf{R}} - \frac{\hbar^2}{2}\left(\frac{1}{m}+\frac{1}{M}\right)\Delta_{\mathbf{r}} \\
&= -\frac{\hbar^2}{2}\left(\frac{M}{(M+m)^2} + \frac{m}{(M+m)^2}\right)\Delta_{\mathbf{R}} - \frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}} \\
&= -\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}} - \frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}}.
\end{aligned}
$$

Let $\varphi(\mathbf{R},\mathbf{r}) = \psi(\mathbf{r}_1(\mathbf{R},\mathbf{r}),\mathbf{r}_2(\mathbf{R},\mathbf{r}))$, therefore we obtain

$$
\boxed{\left(-\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}} - \frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\varphi(\mathbf{R},\mathbf{r}) = E\varphi(\mathbf{R},\mathbf{r})}.
$$

d) Assume that $M \gg m$ and $\frac{1}{m} \gg \frac{1}{M+m}$, then

$$
\begin{aligned}
m^* &= \frac{mM}{M+m} \approx \frac{mM}{M} = m, \\
-\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}} - \frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}} &\approx -\frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}} \approx -\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}.
\end{aligned}
$$

Then, the resulting Schrödinger's equation involving only $\mathbf{r}$ is

$$
\boxed{\left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\varphi(\mathbf{r}) = E\varphi(\mathbf{r})},
$$

where we assume $\mathbf{R}$ is effectively constant.

e) We now take a look at the Schrödinger's equation involving both $\mathbf{R}$ and $\mathbf{r}$

$$
\left(-\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}} - \frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\varphi(\mathbf{R},\mathbf{r}) = E\varphi(\mathbf{R},\mathbf{r})
$$

and assume the solution is separable, i.e., $\varphi(\mathbf{R},\mathbf{r}) = \varphi(\mathbf{r})\chi(\mathbf{R})$, then

$$
\left(-\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}} - \frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\varphi(\mathbf{r})\chi(\mathbf{R}) = E\varphi(\mathbf{r})\chi(\mathbf{R})
$$

or

$$
-\frac{\hbar^2}{2(M+m)}\varphi(\mathbf{r})\Delta_{\mathbf{R}}\chi(\mathbf{R}) - \frac{\hbar^2}{2m^*}\chi(\mathbf{R})\Delta_{\mathbf{r}}\varphi(\mathbf{r}) + V(\mathbf{r})\varphi(\mathbf{r})\chi(\mathbf{R}) = E\varphi(\mathbf{r})\chi(\mathbf{R}).
$$

Dividing the entire equation by $\varphi(\mathbf{r})\chi(\mathbf{R})$ (assuming $\varphi(\mathbf{r})\chi(\mathbf{R}) \neq 0$) we get

$$
\left(-\frac{\hbar^2}{2(M+m)}\frac{1}{\chi(\mathbf{R})}\Delta_{\mathbf{R}}\chi(\mathbf{R})\right) + \left(-\frac{\hbar^2}{2m^*}\frac{1}{\varphi(\mathbf{r})}\Delta_{\mathbf{r}}\varphi(\mathbf{r}) + V(\mathbf{r})\right) = E.
$$

Because each term depends on a different variable, we can only satisfy this equation if each term is constant. We denote the constants $E_{\mathbf{r}}$ and $E_{\mathbf{R}}$, which are required to satisfy $E_{\mathbf{r}} + E_{\mathbf{R}} = E$, then

$$\begin{aligned} -\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}}\chi(\mathbf{R}) + V_{\mathbf{R}}\chi(\mathbf{R}) &= E_{\mathbf{R}}\chi(\mathbf{R}), \\ -\frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}}\varphi(\mathbf{r}) + V(\mathbf{r})\varphi(\mathbf{r}) &= E_{\mathbf{r}}\varphi(\mathbf{r}), \end{aligned}$$

with $V_{\mathbf{R}} = 0$.