CAM 389C Exercise Set II.3

Truman Ellis

November 9, 2010

Problem II.2.7

Which of the following operators are Hermitian?

a) e^{ix}

b) $\dfrac{\mathrm{d}^2}{\mathrm{d}x^2}$

c) $x\dfrac{\mathrm{d}}{\mathrm{d}x}$

Solution

a) An operator Q is Hermitian if

$$\langle u, Qv\rangle = \langle Qu, v\rangle \ .$$

Also, in order to evaluate the inner product, the functions u and v and their derivatives must vanish at $\pm\infty$. Then

$$\left\langle u, \mathrm{e}^{ix} v\right\rangle = \int_{-\infty}^{\infty} u^* \mathrm{e}^{ix} v \, \mathrm{d}x \,,$$

and

$$\left\langle \mathrm{e}^{ix} u, v\right\rangle = \int_{-\infty}^{\infty} \mathrm{e}^{-ix} u^* v \, \mathrm{d}x \,,$$

Clearly these are not going to evaluate identically for all functions $u(x)$ and $v(x)$. Thus, e^{ix} is not a Hermitian operator.

b) Integrating by parts twice,

$$\begin{aligned}
\left\langle u, \frac{\mathrm{d}^2}{\mathrm{d}x^2} v \right\rangle &= \int_{\mathbb{R}} u^* \frac{\mathrm{d}^2 v}{\mathrm{d}x^2}\, \mathrm{d}x \\
&= \cancel{u^*} \frac{\mathrm{d}v}{\mathrm{d}x}\bigg|_0^a - \int_{\mathbb{R}} \frac{\mathrm{d}v}{\mathrm{d}x} \frac{\mathrm{d}u^*}{\mathrm{d}x}\, \mathrm{d}x \\
&= -\frac{\mathrm{d}u^*}{\mathrm{d}x} \cancel{v}\bigg|_0^a + \int_{\mathbb{R}} v \frac{\mathrm{d}^2 u^*}{\mathrm{d}x^2}\, \mathrm{d}x \\
&= \left\langle \frac{\mathrm{d}^2}{\mathrm{d}x^2} u, v \right\rangle .
\end{aligned}$$

Therefore $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ is a Hermitian operator.

c)

$$\begin{aligned}
\left\langle u, x \frac{\mathrm{d}}{\mathrm{d}x} v \right\rangle &= \int_{\mathbb{R}} u^* x \frac{\mathrm{d}v}{\mathrm{d}x}\, \mathrm{d}x && \text{integrate by parts} \\
&= \cancel{u^* x v}\big|_{-\infty}^{\infty} - \int_{\mathbb{R}} x \frac{\mathrm{d}u^*}{\mathrm{d}x} v\, \mathrm{d}x - \int_{\mathbb{R}} u^* v\, \mathrm{d}x \\
&= -\left\langle x \frac{\mathrm{d}}{\mathrm{d}x} u, v \right\rangle - \langle u, v \rangle \neq \left\langle x \frac{\mathrm{d}}{\mathrm{d}x} u, v \right\rangle .
\end{aligned}$$

Therefore,$x\frac{\mathrm{d}}{\mathrm{d}x}$ is not a Hermitian operator.

Problem II.2.8

Ehrenfest's theorem relates the time derivative of the expected value $\langle Q \rangle$ of an operator $\tilde{Q}$ to the commutator $[\tilde{Q}, H]$ of the operator with the Hamiltonian of the system, as follows:

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

Derive the following intermediate results:

a)

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

Solution

We can just use the product rule as follows

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

b)

$$
\frac{\partial \Psi^*}{\partial t} = -\frac{1}{i\hbar} H \Psi^* \,.
$$

Solution

The next result is somewhat trivial. According to the Schrodinger equation,

$$
H\Psi = i\hbar \frac{\partial \Psi}{\partial t} \,.
$$

From this we get

$$
\frac{1}{i\hbar} H\Psi = \frac{\partial \Psi}{\partial t} \,.
$$

Taking the complex conjugate of both sides and noting that H is a Hermitian operator,

$$
-\frac{1}{i\hbar} H\Psi^* = \frac{\partial \Psi^*}{\partial t} \,.
$$

c) Complete the proof of Ehrenfest's theorem.
Substituting our results from **b)** into **a)**,

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

Problem II.3.1

This exercise is designed to carry through the classical method of separation of variables for the solution of partial differential equations. The problem is the two-dimensional *particle in a box*. The physical situation is that of a single particle in a square box $\overline{\Omega} = [0, a] \times [0, b]$ in the xy-plane in a quantum system for which the potential $V = V(x, y)$ is

$$V(x,y) = \begin{cases} 0\,, & \text{for } 0 \le x \le a\,,\; 0 \le y \le b\,, \\ \infty\,, & \text{otherwise}\,. \end{cases}$$

The Hamiltonian is thus

$$H = \begin{cases} (-\hbar^2/2m)\Delta & \text{in the box } \big((x,y) \in \overline{\Omega}\big)\,, \\ +\infty & \text{outside the box,} \end{cases}$$

where Δ is teh two-dimensional Laplacian,

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^y}\,.$$

Thus, the wave function $\Psi = 0$ outside $\overline{\Omega}$. Considering the time-independent Schrodinger equatio, we wish to find $\psi = \psi(x, y)$ satisfying

$$\begin{aligned} H\psi &= E\psi && \text{in } \overline{\Omega}\,, \\ \psi &= 0 && \text{on } \partial\overline{\Omega}\,. \end{aligned}$$

a) Use the standard trick of the method of separation of variables: assume ψ is a product of a function $X(x)$ and a function $Y(y)$: $\psi(x, y) = X(x)Y(y)$, and derive two ordinary differential equations, one for X and one for Y under the assumption that E is the sum, $E = e_X + e_Y$, e_X = constant, e_Y = constant. Show that the solutions are of the form

$$\psi_{nn'}(x,y) = \sqrt{\frac{4}{ab}} \sin\frac{n\pi x}{a} \sin\frac{n'\pi y}{b}\,.$$

Solution

Let us start by plugging $\psi = X(x)Y(y)$ into our governing equation,

$$\begin{aligned} H(XY) - EXY &= -\frac{\hbar^2}{2m}\Delta X(x)Y(y) \\ &= -\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2X(x)}{\mathrm{d}x^2}Y(y) + X(x)\frac{\mathrm{d}^2Y(y)}{\mathrm{d}y^2}\right) - E(X(x)Y(y)) = 0\,. \end{aligned}$$

Now divide by $-\frac{\hbar^2}{2m}XY$,

$$\frac{1}{X}\frac{\mathrm{d}^2X}{\mathrm{d}x^2} + \frac{1}{Y}\frac{\mathrm{d}^2Y}{\mathrm{d}y^2} + \frac{2m}{\hbar^2}E = 0\,.$$

Therefore,

$$-\frac{1}{X}\frac{\mathrm{d}^2X}{\mathrm{d}x^2} = \frac{1}{Y}\frac{\mathrm{d}^2Y}{\mathrm{d}y^2} + \frac{2m}{\hbar^2}E\,.$$

Since one side of the equation is strictly a function of x and the other side is strictly a function of y, they must both be equal to a constant e_X. Solving the X equation first:

$$\frac{\mathrm{d}^2X}{\mathrm{d}x^2} + e_X X = 0\,.$$

The zero boundary conditions eliminate the possibility of a polynomial solution to this ODE and stipulate that e_X must be positive, otherwise the solution would involve terms of the form $X = A\mathrm{e}^{\sqrt{-e_X}x}$ which obviously can not be zero at the boundaries (neglecting the trivial case of $A = 0$). Therefore our solution must be of the form

$$X(x) = A\cos(\sqrt{e_X}x) + B\sin(\sqrt{e_X}x)\,.$$

Applying the boundary conditions

$$X(0) = A = 0\,,$$

and

$$X(a) = B\sin(\sqrt{e_X}a) = 0\,.$$

Thus either $B = 0$ (trivial) or $\sqrt{e_X}a = n\pi$. Taking the non-trivial case, $e_X = \frac{n^2\pi^2}{a^2}$.
Therefore,

$$X(x) = B\sin\left(\frac{n\pi x}{a}\right)\,.$$

Turning to the Y equation,

$$\frac{1}{Y}\frac{\mathrm{d}^2Y}{\mathrm{d}y^2} + \frac{2m}{\hbar^2}E = \frac{n^2\pi^2}{a^2}\,.$$

Rearranging terms,

$$\frac{\mathrm{d}^2Y}{\mathrm{d}y^2} = \left(\frac{n^2\pi^2}{a^2} - \frac{2m}{\hbar^2}E\right)Y = e_Y Y$$

By similar argument from before, e_Y must be positive and $Y(y)$ must be of the form

$$Y(y) = C\cos(\sqrt{e_Y}y) + D\sin(\sqrt{e_Y}y)\,.$$

Applying the boundary conditions,

$$Y(0) = c = 0\,,$$

and

$$Y(b) = D\sin(\sqrt{e_Y}y) = 0\,.$$

And by similar argument as before,

$$e_Y = \frac{n'^2\pi^2}{b^2}\,.$$

So,

$$Y(y) = D\sin\left(\frac{n'\pi y}{b}\right)\,.$$

But $\psi_{nn'}(x,y) = X(x)Y(y) = BD\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{n'\pi y}{b}\right)$ must be normalized, so

$$\left\langle BD\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{n'\pi y}{b}\right), BD\sin\left(\frac{p\pi x}{a}\right)\sin\left(\frac{p'\pi y}{b}\right)\right\rangle$$
$$= \begin{cases} B^2D^2\frac{ab}{4}\,, & n = p \text{ and } n' = p'\,, \\ 0\,, & \text{else}\,. \end{cases}$$

Therefore, $BD = \sqrt{\frac{4}{ab}}$, and

$$\psi_{nn'}(x,y) = \sqrt{\frac{4}{ab}}\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{n'\pi y}{b}\right)\,.$$

b) Show that the energy levels are given by

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

Solution

From before,

$$e_Y = \frac{n'^2\pi^2}{b^2} = \frac{n^2\pi^2}{a^2} - \frac{2m}{\hbar^2}E\,,$$

and isolating E,

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

c) For the case of a square box, $(a = b)$, determine the energy levels $\mu = \dfrac{\hbar^2\pi^2}{2ma^2}(n^2 + n'^2)$ for values of n and n' up to 4. What is the lowest energy level of the system?

Solution

The calculation is straightforward, just plug in values for n and n' into the formula for the energy levels. The table below demonstrates the possible energy levels. Clearly the lowest energy level corresponds to $n = n' = 1$, $\mu_{11} = \dfrac{\hbar^2\pi^2}{ma^2}$.

Table 1: Possible energy levels for square box

		n			
		1	2	3	4
n'	1	$\frac{\hbar^2\pi^2}{ma^2}$	$2.5\frac{\hbar^2\pi^2}{ma^2}$	$5\frac{\hbar^2\pi^2}{ma^2}$	$8.5\frac{\hbar^2\pi^2}{ma^2}$
	2	$2.5\frac{\hbar^2\pi^2}{ma^2}$	$4\frac{\hbar^2\pi^2}{ma^2}$	$6.5\frac{\hbar^2\pi^2}{ma^2}$	$10\frac{\hbar^2\pi^2}{ma^2}$
	3	$5\frac{\hbar^2\pi^2}{ma^2}$	$6.5\frac{\hbar^2\pi^2}{ma^2}$	$9\frac{\hbar^2\pi^2}{ma^2}$	$12.5\frac{\hbar^2\pi^2}{ma^2}$
	4	$8.5\frac{\hbar^2\pi^2}{ma^2}$	$10\frac{\hbar^2\pi^2}{ma^2}$	$12.5\frac{\hbar^2\pi^2}{ma^2}$	$16\frac{\hbar^2\pi^2}{ma^2}$

Problem II.3.2

This exercise concerns a well-known argument for using the nucleus of the hydrogen atom as the origin of the coordinate system as opposed to the center of mass. The situation is this: the quantum system of two particles, particle 1 of mass M (corresponding, e.g., to the nucleus) and particle 2 of mass m (e.g. the electron), with origin at a point O. The particles are located at positions $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. The center of mass is located at $\mathbf{R} = (\mathbf{r}_1 M + \mathbf{r}_2)/(M+m)$ and the vector connecting 1 to 2 is $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. The goal is to rederive Schrodinger's equations with a change of variables from $(\mathbf{r}_1, \mathbf{r}_2)$ to $(\mathbf{R}, \mathbf{r})$.

a) Show that

$$\mathbf{r}_1 = \mathbf{R} + \frac{m^*}{M}\mathbf{r} \quad \text{and} \quad \mathbf{r}_2 = \mathbf{R} - \frac{m^*}{M}\mathbf{r}\,,$$

where $m^* = Mm/(M+m)$.

Solution

Substituting $\mathbf{r}_2 = \mathbf{r}_1 - \mathbf{r}$ into $\mathbf{R} = \frac{\mathbf{r}_1 M + \mathbf{r}_2 m}{M+m}$,

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

Then

$$\begin{aligned}\mathbf{r}_1 &= \frac{(M+m)\mathbf{R} + m\mathbf{r}}{M+m} = \mathbf{R} + \frac{m}{M+m}\mathbf{r} = \mathbf{R} + \frac{Mm}{M(M+m)}\mathbf{r} \\ &= \mathbf{R} + \frac{m^*}{m}\mathbf{r}\,.\end{aligned}$$

From the fact that $\mathbf{r}_2 = \mathbf{r}_1 - \mathbf{r}$,

$$\begin{aligned}
\mathbf{r}_2 &= \mathbf{R} + \frac{m}{M+m}\mathbf{r} - \frac{M+m}{M+m}\mathbf{r} = \mathbf{R} + \left(\frac{m-M-m}{M+m}\right)\mathbf{r} \\
&= \mathbf{R} - \frac{mM}{m(M+m)}\mathbf{r} \\
&= \mathbf{R} - \frac{m^*}{m}\mathbf{r}\,.
\end{aligned}$$

b) Using the change of variables, show that

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

Solution

First note that

$$\begin{array}{cc}
\frac{\partial \mathbf{R}}{\partial \mathbf{r}_1} = \frac{M}{M+m} = \frac{m^*}{m} & \frac{\partial \mathbf{R}}{\partial \mathbf{r}_2} = \frac{m}{M+m} = \frac{m^*}{M} \\
\frac{\partial \mathbf{r}}{\partial \mathbf{r}_1} = 1 & \frac{\partial \mathbf{r}}{\partial \mathbf{r}_2} = -1\,.
\end{array}$$

Then,

$$\frac{\partial}{\partial \mathbf{r}_1} = \frac{\partial}{\partial \mathbf{R}}\frac{\partial \mathbf{R}}{\partial \mathbf{r}_1} + \frac{\partial}{\partial \mathbf{r}}\frac{\partial \mathbf{r}}{\partial \mathbf{r}_1} = \frac{m^*}{m}\frac{\partial}{\partial \mathbf{R}} + \frac{\partial}{\partial \mathbf{r}}\,.$$

Similarly

$$\frac{\partial}{\partial \mathbf{r}_2} = \frac{\partial}{\partial \mathbf{R}}\frac{\partial \mathbf{R}}{\partial \mathbf{r}_2} + \frac{\partial}{\partial \mathbf{r}}\frac{\partial \mathbf{r}}{\partial \mathbf{r}_2} = \frac{m^*}{M}\frac{\partial}{\partial \mathbf{R}} - \frac{\partial}{\partial \mathbf{r}}\,.$$

But $\nabla_{\mathbf{r}_1} = \mathbf{e}_i \frac{\partial}{\partial \mathbf{r}_{1i}}$, and similarly for $\mathbf{r}_2$, $\mathbf{r}$, and $\mathbf{R}$. Therefore,

$$\nabla_{\mathbf{r}_1} = \frac{m^*}{m}\nabla_{\mathbf{R}} + \nabla_{\mathbf{r}}$$

and

$$\nabla_{\mathbf{r}_2} = \frac{m^*}{M}\nabla_{\mathbf{R}} - \nabla_{\mathbf{r}}\,.$$

c) Show that, in these new variables, the time-independent Schrodinger equation is:

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

Solution

We first need to derive the Laplacian operator in our changed coordinates. So,

$$\Delta_{\mathbf{r}_1} = \frac{\partial}{\partial \mathbf{r}_1}\cdot\frac{\partial}{\partial \mathbf{r}_1} = \left(\frac{m^*}{m}\right)^2\Delta_{\mathbf{R}} + 2\left(\frac{m^*}{m}\right)\Delta_{\mathbf{rR}} + \Delta_{\mathbf{r}}$$

and

$$\Delta_{\mathbf{r}_2} = \frac{\partial}{\partial \mathbf{r}_2} \cdot \frac{\partial}{\partial \mathbf{r}_2} = \left(\frac{m^*}{M}\right)^2 \Delta_{\mathbf{R}} - 2\left(\frac{m^*}{M}\right)\Delta_{\mathbf{rR}} + \Delta_{\mathbf{r}}$$

We can write the time independent Schrodinger's equation as

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

Substituting our expressions for $\Delta_{\mathbf{r}_1}$ and $\Delta_{\mathbf{r}_2}$,

$$\begin{aligned}
&\left(-\frac{\hbar^2}{2M}\left(\left(\frac{m^*}{m}\right)^2 \Delta_{\mathbf{R}} + \cancel{2\left(\frac{m^*}{m}\right)\Delta_{\mathbf{rR}}} + \Delta_{\mathbf{r}}\right)\right.\\
&\left.-\frac{\hbar^2}{2m}\left(\left(\frac{m^*}{M}\right)^2 \Delta_{\mathbf{R}} - \cancel{2\left(\frac{m^*}{M}\right)\Delta_{\mathbf{rR}}} + \Delta_{\mathbf{r}}\right) + V(\mathbf{r})\right)\psi\\
&= \left(-\frac{\hbar^2 m^{*2}}{2Mm}\left(\frac{1}{m} + \frac{1}{M}\right)\Delta_{\mathbf{R}} - \frac{\hbar^2}{2}\left(\frac{1}{m} + \frac{1}{M}\right)\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\psi\\
&= \left(-\frac{\hbar^2 m^{*\cancelto{1}{2}}}{2Mm}\cancel{\left(\frac{M+m}{Mm}\right)}\Delta_{\mathbf{R}} - \frac{\hbar^2}{2}\left(\frac{M+m}{mM}\right)\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\psi\\
&= \left(-\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}} - \frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\psi = E\psi\,.
\end{aligned}$$

d) Now if $M \gg m$ so that $M + m \approx M$ and $1/m \gg 1/(M+m)$, write down the resulting approximate Schrodinger equation involving only $\mathbf{r}$.

Solution

$$\begin{aligned}
&\left(-\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}} - \frac{\hbar^2(M+m)}{2Mm}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\psi\\
&\approx \left(-\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}} - \frac{\hbar^2\cancel{M}}{2\cancel{M}m}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\psi\\
&= \left(-\underbrace{\frac{\hbar^2}{2(M+m)}}_{\ll \frac{\hbar^2}{2m}}\Delta_{\mathbf{R}} - \frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\psi\\
&\approx \left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r})\right)\psi = E\psi\,.
\end{aligned}$$

e) Suppose now that the wave function is separable:$\psi(\mathbf{r}, \mathbf{R}) = \psi(\mathbf{r})\chi(\mathbf{R})$. Show that χ satisfies the one-particle Schrodinger equation with mass $M + m$, with potential $V_{\mathbf{R}} = 0$, and energy $E_{\mathbf{R}}$, while ψ satisfies the one-particle Schrodinger equation with mass m^* and potential $V(\mathbf{r})$, and energy $E_{\mathbf{r}}$, with the total energy $E = E_{\mathbf{R}} + E_{\mathbf{r}}$.

Solution

Substituting our separated wave function into the Schrodinger equation,

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

Dividing by $\psi(\mathbf{r})\chi(\mathbf{R})$ and separating variables,

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

Since the left hand side is strictly a function of $\mathbf{R}$ and the right hand side is strictly a function of $\mathbf{r}$, both sides must be equal to a constant. Also, assuming we have split split up our energy appropriately, the constant must be zero. Expanding the left hand side,

$$-\frac{\hbar^2}{2(M+m)}\Delta_{\mathbf{R}}\chi(\mathbf{R}) = E_{\mathbf{R}}\chi(\mathbf{R})\,,$$

which is precisely the one-dimensional Schrodinger equation with mass $M + m$, potential $V_{\mathbf{R}} = 0$, and energy $E_{\mathbf{R}}$. Similarly with the right hand side,

$$-\frac{\hbar^2}{2m^*}\Delta_{\mathbf{r}}\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E_{\mathbf{r}}\psi(\mathbf{r})\,,$$

which is the one-dimensional Schrodinger equation with mass m^*, potential $V(\mathbf{r})$, and energy $E_{\mathbf{r}}$.