Coláiste na Tríonóide, Baile Átha Cliath
Trinity College Dublin
Ollscoil Átha Cliath | The University of Dublin

Faculty of Science, Technology, Engineering and Mathematics

School of Mathematics

JS Mathematics **Michaelmas Term 2023**
JS Theoretical Physics

Module MAU34403: Quantum Mechanics I

Wednesday ? 29? December 2023 RDS Simmonscourt? 14.00 — 16.00?

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Instructions to candidates:

Attempt all questions.

Each question is worth 33 marks.

Additional instructions for this examination:

Formulae and Tables are available from the invigilators, if required.

Non-programmable calculators are permitted for this examination,—please indicate the make and model of your calculator on each answer book used.

You may not start this examination until you are instructed to do so by the Invigilator.

1. The XXX Heisenberg spin-1/2 chain of length 2 is described by the Hamiltonian

$$H = \frac{3}{4}J + \frac{J}{\hbar^2}\sum_{\alpha=1}^{3} S_1^\alpha S_2^\alpha$$

which acts on the tensor product of 2 copies of $\mathbb{C}^2$ (spin up-down) $\mathscr{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$.

The spin-1/2 operator S_i^α acts only at the i-th site

$$S_1^\alpha = S^\alpha \otimes I\,, \quad S_2^\alpha = I \otimes S^\alpha\,, \quad S^\alpha = \hbar\sigma^\alpha/2\,.$$

The Hamiltonian commutes with the total spin operator

$$\mathbb{S}^\alpha = S_1^\alpha + S_2^\alpha = S^\alpha \otimes I + I \otimes S^\alpha$$

(a) **6 marks.** Show that the orthonormal vectors

$$|e_1\rangle \equiv |\uparrow\uparrow\rangle\,, \quad |e_0\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\,, \quad |e_{-1}\rangle \equiv |\downarrow\downarrow\rangle\,, \quad |f\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

are eigenvectors of H with the eigenvalues $E_1 = J$ and $E_0 = 0$. Show that they are also eigenvectors of $\mathbb{S}^3$ with eigenvalues $s_1 = \hbar$, $s_0 = 0$, and $s_{-1} = -\hbar$.

(b) Consider the state

$$|\psi\rangle = \frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle + 2\,\mathrm{i}\,|\uparrow\downarrow\rangle - \mathrm{i}\,|\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big)$$

i. **6 marks.** Expand $|\psi\rangle$ over the basis $|f\rangle$ and $|e_m\rangle$, $m = 1, 0, -1$.

Find the probabilities to measure E_0 and E_1, and s_1, s_0 and s_{-1}.

Answer. We compute

$$\begin{aligned}
\langle e_1|\psi\rangle &= \langle\uparrow\uparrow|\frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle + 2\mathrm{i}|\uparrow\downarrow\rangle - \mathrm{i}|\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big) = \frac{1}{\sqrt{10}} \\
\langle e_0|\psi\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle + 2\mathrm{i}|\uparrow\downarrow\rangle - \mathrm{i}|\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big) = \frac{1}{\sqrt{20}}(2\mathrm{i} - \mathrm{i}) = \frac{\mathrm{i}}{\sqrt{20}} \\
\langle e_{-1}|\psi\rangle &= \langle\downarrow\downarrow|\frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle + 2\mathrm{i}|\uparrow\downarrow\rangle - \mathrm{i}|\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big) = \frac{2}{\sqrt{10}} \\
\langle f|\psi\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle + 2\mathrm{i}|\uparrow\downarrow\rangle - \mathrm{i}|\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big) = \frac{1}{\sqrt{20}}(2\mathrm{i} + \mathrm{i}) = \frac{3\mathrm{i}}{\sqrt{20}}
\end{aligned} \tag{1}$$

Thus,

$$\begin{aligned}
|\psi\rangle &= |e_1\rangle\langle e_1|\psi\rangle + |e_0\rangle\langle e_0|\psi\rangle + |e_{-1}\rangle\langle e_{-1}|\psi\rangle + |f\rangle\langle f|\psi\rangle \\
&= \frac{1}{\sqrt{10}}|e_1\rangle + \frac{\mathrm{i}}{\sqrt{20}}|e_0\rangle + \frac{2}{\sqrt{10}}|e_{-1}\rangle + \frac{3\mathrm{i}}{\sqrt{20}}|f\rangle
\end{aligned} \tag{2}$$

and

$$P(E_1) = \frac{1}{10} + \frac{1}{20} + \frac{4}{10} = \frac{11}{20}\,, \quad P(E_0) = \frac{9}{20} \tag{3}$$

$$P(s_1) = \frac{1}{10}\,, \quad P(s_0) = \frac{1}{20} + \frac{9}{20} = \frac{1}{2}\,, \quad P(s_{-1}) = \frac{4}{10} = \frac{2}{5} \tag{4}$$

ii. **5 marks.** If the result of a measurement of H on $|\psi\rangle$ is E_1, what is the state of the system after it? If the result of a measurement $\mathbb{S}^3$ on $|\psi\rangle$ is s_0, what is the state of the system after it?

Answer. After the measurements the system collapses into

$$\begin{aligned}|\mathcal{E}_1\rangle &= \frac{|e_1\rangle\langle e_1|\psi\rangle + |e_0\rangle\langle e_0|\psi\rangle + |e_{-1}\rangle\langle e_{-1}|\psi\rangle}{\sqrt{P(E_1)}} = \sqrt{\frac{20}{11}}\big(\frac{1}{\sqrt{10}}|e_1\rangle + \frac{\mathrm{i}}{\sqrt{20}}|e_0\rangle + \frac{2}{\sqrt{10}}|e_{-1}\rangle\big) \\ &= \sqrt{\frac{2}{11}}|e_1\rangle + \frac{\mathrm{i}}{\sqrt{11}}|e_0\rangle + \sqrt{\frac{8}{11}}|e_{-1}\rangle\end{aligned} \tag{5}$$

$$\begin{aligned}|s_0\rangle &= \frac{|e_0\rangle\langle e_0|\psi\rangle + |f\rangle\langle f|\psi\rangle}{\sqrt{P(s_0)}} = \sqrt{2}\big(\frac{\mathrm{i}}{\sqrt{20}}|e_0\rangle + \frac{3\mathrm{i}}{\sqrt{20}}|f\rangle\big) \\ &= \frac{\mathrm{i}}{\sqrt{10}}|e_0\rangle + \frac{3\mathrm{i}}{\sqrt{10}}|f\rangle\end{aligned} \tag{6}$$

iii. **5 marks.** What is the probability to measure first E_1 and immediately after s_0? What is the probability to measure first s_0 and immediately after E_1? Are these probabilities equal? Explain the result.

Answer. The probability to find s_0 by measuring $|\mathcal{E}_1\rangle$ is $|\langle e_0|\mathcal{E}_1\rangle|^2 = 1/11$. The probabilities multiply, so

$$P(E_1, s_0) = P(E_1)|\langle e_0|\mathcal{E}_1\rangle|^2 = \frac{1}{20} \tag{7}$$

Similarly,

$$P(s_0, E_1) = P(s_0)|\langle e_0|s_0\rangle|^2 = \frac{1}{20} \tag{8}$$

They are equal because H and $\mathbb{S}^3$ are compatible.

iv. **6 marks.** Find the expectation values of and the uncertainty in the Hamiltonian H and the z-component $\mathbb{S}^3$ of the total spin operator with respect to $|\psi\rangle$

Answer. We get

$$\langle H\rangle = P(E_0)E_0 + P(E_1)E_1 = \frac{9}{20}0 + \frac{11}{20}J = \frac{11}{20}J \tag{9}$$

$$\Delta H = \sqrt{P(E_0)(E_0-\langle H\rangle)^2 + P(E_1)(E_1-\langle H\rangle)^2} = J\sqrt{\frac{9}{20}\frac{11^2}{20^2} + \frac{11}{20}(1-\frac{11}{20})^2} = \frac{3\sqrt{11}}{20}J \tag{10}$$

$$\langle \mathbb{S}^3\rangle = P(s_1)s_1 + P(s_0)s_0 + P(s_{-1})s_{-1} = \frac{1}{10} + \frac{1}{2}0 + \frac{2}{5}(-1) = -\frac{3\hbar}{10} \tag{11}$$

$$\Delta\mathbb{S}^3 = \sqrt{P(s_1)(s_1-\langle\mathbb{S}^3\rangle)^2 + P(s_0)(s_0-\langle\mathbb{S}^3\rangle)^2 + P(s_{-1})(s_{-1}-\langle\mathbb{S}^3\rangle)^2} := \frac{\hbar\sqrt{41}}{10} \tag{12}$$

v. **5 marks.** Compute $\langle\mathbb{S}^3\, H\rangle$ and $\langle H\,\mathbb{S}^3\rangle$, and check that the general uncertainty relation

$$\Delta\hat{A}^2\Delta\hat{B}^2 \geq \Big(\frac{1}{2}\langle[\hat{A}\,,\,\hat{B}]_+\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle\Big)^2 - \frac{1}{4}\langle[\hat{A}\,,\,\hat{B}]\rangle^2$$

holds for $\mathbb{S}^3$ and H.

Answer. Since $\mathbb{S}^3$ and H commute the rhs of the general uncertainty relation gives

$$\Big(\langle\mathbb{S}^3\,H\rangle - \langle\mathbb{S}^3\rangle\langle H\rangle\Big)^2 \tag{13}$$

Then,

$$\begin{aligned}\langle\mathbb{S}^3\,H\rangle = \langle H\,\mathbb{S}^3\rangle &= \langle\psi|\mathbb{S}^3\,H\left(\frac{1}{\sqrt{10}}|e_1\rangle + \frac{\mathrm{i}}{\sqrt{20}}|e_0\rangle + \frac{2}{\sqrt{10}}|e_{-1}\rangle + \frac{3\mathrm{i}}{\sqrt{20}}|f\rangle\right)\\ &= \langle\psi|\mathbb{S}^3\,J\left(\frac{1}{\sqrt{10}}|e_1\rangle + \frac{\mathrm{i}}{\sqrt{20}}|e_0\rangle + \frac{2}{\sqrt{10}}|e_{-1}\rangle\right)\\ &= \hbar J\langle\psi|\left(\frac{1}{\sqrt{10}}|e_1\rangle - \frac{2}{\sqrt{10}}|e_{-1}\rangle\right) = -\frac{3\hbar J}{10}\end{aligned} \tag{14}$$

Thus,

$$\Big(\langle\mathbb{S}^3\,H\rangle - \langle\mathbb{S}^3\rangle\langle H\rangle\Big)^2 = (\frac{3\hbar J}{10} - \frac{3\hbar}{10}\frac{11}{20}J)^2 \approx 0.018225\hbar^2J^2 \tag{15}$$

$$\Delta H^2 = \frac{99}{20^2}J^2\,,\quad (\Delta\mathbb{S}^3)^2 = \frac{\hbar^2 41}{100}\,,\quad \Delta H^2(\Delta\mathbb{S}^3)^2 \approx 0.101475\hbar^2J^2 \tag{16}$$

and the inequality holds.

2. Consider a particle in the following potential

$$V(x) = -\nu\delta(x+a) - \nu\delta(x-a)\,,$$

where $a > 0\,,\ \nu > 0$.

(a) **3 marks.** Show that the wave eigenfunctions of the Hamiltonian H can always be chosen to be either even or odd.

Solution: Since the potential is even, H commutes with the parity operator $\mathcal{P}$, and therefore one can choose a common basis of eigenstates of H and $\mathcal{P}$. Since $\mathcal{P}^2 = 1$ the eigenvalues of the parity operator can only be ± 1, and the corresponding wave functions are either even (for $+1$) or odd.

(b) **Even parity states**

i. **5 marks.** Find an even wave function for a bound state. Do not normalise the wave function. Sketch a plot of the wave function by setting $a = 1$, $\kappa = 1$ where $\kappa = \frac{\sqrt{-2mE}}{\hbar}$, and choosing any normalisation of the wave function.

Solution: The time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\psi'' + V(x)\psi = E\psi\,. \tag{17}$$

By using the Heaviside function we can write any function $\psi(x)$ in the form

$$\psi(x) = \psi_L(x)\theta(-x-a) + \psi_M(x)(\theta(x+a) - \theta(x-a)) + \psi_R(x)\theta(x-a)\,. \tag{18}$$

$\psi(x)$ is even, $\psi(-x) = \psi(x)$, therefore $\psi_L(-x) = \psi_R(x)\,,\ \psi_M(-x) = \psi_M(x)$. Since $V(x) = 0$ for all x except $x = \pm a$, we need to glue the following three solutions of the time-independent Schrödinger equation

$$\begin{aligned}
\psi_L(x) &= Be^{+\kappa\,(x+a)}\,, \quad x < -a\,,\\
\psi_R(x) &= Be^{-\kappa\,(x-a)}\,, \quad x > a\,,\\
\psi_M(x) &= A\cosh(\kappa\, x)\,, \quad -a < x < a\,, \quad \kappa = \frac{\sqrt{-2mE}}{\hbar}
\end{aligned} \tag{19}$$

where $E < 0$, and we used that $\psi_L(-\infty) = \psi_R(+\infty) = 0$, and that the wave function is even.

The constant B is expressed in terms of A by using the continuity condition for $\psi(x)$ at $x = a$

$$B = A\cosh(\kappa\, a)\,. \tag{20}$$

Thus, the wave function is given by

$$\begin{aligned}
\psi_L(x) &= A\cosh(\kappa\, a)e^{+\kappa\,(x+a)}\,, \quad x < -a\,,\\
\psi_R(x) &= A\cosh(\kappa\, a)e^{-\kappa\,(x-a)}\,, \quad x > a\,,\\
\psi_M(x) &= A\cosh(\kappa\, x)\,, \quad -a < x < a\,, \quad \kappa = \frac{\sqrt{-2mE}}{\hbar}\,.
\end{aligned} \tag{21}$$

ii. **5 marks.** Find the quantisation condition for even parity states.

Solution:

To find the quantisation condition for the bound state spectrum we compute

$$\begin{aligned}
\psi'(x) &= \psi_L'(x)\theta(-x-a) + \psi_M'(x)(\theta(x+a) - \theta(x-a)) + \psi_R'(x)\theta(x-a)\,,\\
\psi''(x) &= \psi_L''(x)\theta(-x-a) + \psi_M''(x)(\theta(x+a) - \theta(x-a)) + \psi_R''(x)\theta(x-a)\\
&\quad - \psi_L'(-a)\delta(-x-a) + \psi_M'(-a)\delta(x+a) - \psi_M'(a)\delta(x-a) + \psi_R'(a)\delta(x-a)\,.
\end{aligned} \tag{22}$$

Substituting ψ'' in the TISE, we get the following relation between $\psi_M'(a)$ and $\psi_R'(a)$

$$\psi_R'(a) - \psi_M'(a) + \frac{2m\nu}{\hbar^2}\psi_R(a) = 0\,, \tag{23}$$

and therefore

$$\begin{aligned}
&-\kappa\,\cosh(\kappa\, a) - \kappa\,\sinh(\kappa\, a) + \frac{2m\nu}{\hbar^2}\cosh(\kappa\, a) = 0\,,\\
&-\kappa e^{\kappa a} + \frac{m\nu}{\hbar^2}e^{\kappa a} + \frac{m\nu}{\hbar^2}e^{-\kappa a} = 0\,.
\end{aligned} \tag{24}$$

Thus, the quantisation condition is

$$\frac{\hbar^2\kappa}{m\nu} - 1 = e^{-2\kappa a}\,. \tag{25}$$

iii. **5 marks.** Show that for any a and ν there is only one solution to the energy quantisation condition for even parity states. Introduce $W = \frac{m\nu\, a}{\hbar^2}$, and find the leading term in the expansion of $\kappa = \frac{\sqrt{-2mE}}{\hbar}$ for $W \ll 1$ and for $W \gg 1$. Explain the results obtained.

Solution: The lhs of the energy quantisation condition is an increasing function of κ with the negative value -1 at $\kappa = 0$. The rhs is a decreasing positive function. Thus, their graphs always intersect at one point.

In terms of W the energy quantisation condition takes the form

$$\kappa a = W + W e^{-2\kappa a} \,. \tag{26}$$

Thus,

$$\kappa a = 2W - 4W^2 + \cdots \,, \quad \text{for } \; W \ll 1 \,, \tag{27}$$

and

$$\kappa a = W + W e^{-2W} + \cdots \,, \quad \text{for } \; W \gg 1 \,. \tag{28}$$

These are ground state energies of a particle in the potential $-2\nu\delta(x)$ and $-\nu\delta(x)$, respectively. For $W \ll 1$ the ground state wave function is approaching the one for a particle in the potential $-2\nu\delta(x)$. For $W \gg 1$ the wave function in the vicinity of $x = \pm a$ is approaching the one for a particle in the potential $-\nu\delta(x \pm a)$.

(c) **Odd parity states**

i. **5 marks.** Find an odd wave function for a bound state. Do not normalise the wave function. Sketch a plot of the wave function by setting $a = 1$, $\kappa = 1$ where $\kappa = \frac{\sqrt{-2mE}}{\hbar}$, and choosing any normalisation of the wave function.

Solution: The time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\psi'' + V(x)\psi = E\psi \,, \tag{29}$$

By using the Heaviside function we can write any function $\psi(x)$ in the form

$$\psi(x) = \psi_L(x)\theta(-x-a) + \psi_M(x)(\theta(x+a) - \theta(x-a)) + \psi_R(x)\theta(x-a) \,. \tag{30}$$

$\psi(x)$ is odd, $\psi(-x) = -\psi(x)$, therefore

$\psi_L(-x) = -\psi_R(x)\,,\; \psi_M(-x) = -\psi_M(x)$.

Since $V(x) = 0$ for all x except $x = \pm a$, we need to glue the following three solutions of the time-independent Schrödinger equation

$$\begin{aligned} \psi_L(x) &= -Be^{+\kappa\,(x+a)}\,, \quad x < -a\,, \\ \psi_R(x) &= Be^{-\kappa\,(x-a)}\,, \quad x > a\,, \\ \psi_M(x) &= A\sinh(\kappa\,x)\,, \quad -a < x < a\,, \quad \kappa = \frac{\sqrt{-2mE}}{\hbar} \end{aligned} \tag{31}$$

where $E < 0$, and we used that $\psi_L(-\infty) = \psi_R(+\infty) = 0$, and that the wave function is odd.

The constant B is expressed in terms of A by using the continuity condition for $\psi(x)$ at $x = a$

$$B = A\sinh(\kappa\,a)\,. \tag{32}$$

Thus, the wave function is given by

$$\begin{aligned} \psi_L(x) &= -A\sinh(\kappa\,a)e^{+\kappa\,(x+a)}\,, \quad x < -a\,, \\ \psi_R(x) &= A\sinh(\kappa\,a)e^{-\kappa\,(x-a)}\,, \quad x > a\,, \\ \psi_M(x) &= A\sinh(\kappa\,x)\,, \quad -a < x < a\,, \quad \kappa = \frac{\sqrt{-2mE}}{\hbar}\,. \end{aligned} \tag{33}$$

ii. **5 marks.** Find the quantisation condition for odd parity states.

Solution:

To find the quantisation condition for the bound state spectrum we compute

$$\begin{aligned} \psi'(x) &= \psi_L'(x)\theta(-x-a) + \psi_M'(x)(\theta(x+a) - \theta(x-a)) + \psi_R'(x)\theta(x-a)\,, \\ \psi''(x) &= \psi_L''(x)\theta(-x-a) + \psi_M''(x)(\theta(x+a) - \theta(x-a)) + \psi_R''(x)\theta(x-a) \\ &\quad - \psi_L'(-a)\delta(-x-a) + \psi_M'(-a)\delta(x+a) - \psi_M'(a)\delta(x-a) + \psi_R'(a)\delta(x-a)\,. \end{aligned} \tag{34}$$

Substituting ψ'' in the TISE, we get the following relation between $\psi_M'(a)$ and $\psi_R'(a)$

$$\psi_R'(a) - \psi_M'(a) + \frac{2m\nu}{\hbar^2}\psi_R(a) = 0\,, \tag{35}$$

and therefore

$$\begin{aligned} &-\kappa\,\sinh(\kappa\,a) - \kappa\,\cosh(\kappa\,a) + \frac{2m\nu}{\hbar^2}\sinh(\kappa\,a) = 0\,, \\ &-\kappa e^{\kappa a} + \frac{m\nu}{\hbar^2}e^{\kappa a} - \frac{m\nu}{\hbar^2}e^{-\kappa a} = 0\,. \end{aligned} \tag{36}$$

Thus, the quantisation condition is

$$\frac{\hbar^2\kappa}{m\nu} - 1 = -e^{-2\kappa a}\,. \tag{37}$$

iii. **5 marks.** Find all values of $W = \frac{m\nu\, a}{\hbar^2}$ for which there is a solution to the energy quantisation condition for odd parity states, and show that it is the only solution.

Solution: In terms of W the energy quantisation condition takes the form

$$z = W - We^{-2z}\,,\quad z = \kappa a\,. \tag{38}$$

Both the lhs and rhs functions are increasing and equal to 0 at $z = 0$. The rhs function is concaved down and asymptotes to W as $z \to \infty$ while the lhs function is linear and goes to infinity. Therefore, the graphs of these functions will intersect at a single point $z > 0$ only if the slope of the lhs function at $z = 0$ is smaller than the slope of the rhs function. Thus,

$$1 < 2W \quad\Rightarrow\quad W > \frac{1}{2}\,. \tag{39}$$

3. The motion of two particles in one dimension is described by the Hamiltonian

$$H = \frac{P_1^2}{2m} + \frac{P_1P_2}{m_{12}} + \frac{P_2^2}{2m} - 2k\,X_1X_2 + V(X_1+X_2)\,,\quad m>0\,,\ m_{12}>0\,,\ k>0\,,$$

where the potential V is given by

$$V(X) = \begin{cases} +\infty & \text{for } X < 0 \\ k\,X^2/2 & \text{for } 0 < X < a \\ +\infty & \text{for } X > a \end{cases}$$

Pay attention to the plus sign in $V(X_1+X_2)$!

(a) **10 marks.** Introduce the centre of mass coordinate $X_{\rm cm}$ for two particles of the same mass, the relative coordinate X, and their conjugate momenta. Check that they satisfy the canonical commutation relations. How many independent relations do you need to check?

Express the Hamiltonian in terms of the new coordinates and momenta. In classical mechanics for which values of m_{12} and m is the energy of the system positive unless it is at rest?

Answer. We introduce the centre of mass coordinate $X_{\rm cm}$, the relative coordinate X, and their conjugate momenta

$$X_{\rm cm} = \frac{1}{2}X_1 + \frac{1}{2}X_2\,, \quad X = X_1 - X_2\,, \quad P_{\rm cm} = P_1 + P_2\,, \quad P = \frac{1}{2}P_1 - \frac{1}{2}P_2 \tag{40}$$

The new coordinates and momenta satisfy the canonical commutation relations.

The Hamiltonian takes the form

$$\begin{aligned} H &= \frac{P_1^2}{2m} + \frac{P_1P_2}{m_{12}} + \frac{P_2^2}{2m} - 2k\,X_1X_2 + V(X_1+X_2) \\ &= \frac{(P+P_{\rm cm}/2)^2}{2m} - \frac{(P+P_{\rm cm}/2)(P-P_{\rm cm}/2)}{m_{12}} + \frac{(P-P_{\rm cm}/2)^2}{2m} - 2k\,X_{\rm cm}^2 + \frac{kX^2}{2} + V(2X_{\rm cm}) \\ &= \frac{m+m_{12}}{2mm_{12}}\frac{P_{\rm cm}^2}{2} + \frac{2(m_{12}-m)}{mm_{12}}\frac{P^2}{2} - 2k\,X_{\rm cm}^2 + \frac{kX^2}{2} + V(2X_{\rm cm}) = H_{\rm cm} + H_{\rm rel}\,, \end{aligned} \tag{41}$$

where

$$\begin{aligned} &H_{\rm cm} = \frac{P_{\rm cm}^2}{2m_{\rm cm}} + V_{\rm cm}(X_{\rm cm})\,, \quad m_{\rm cm} = \frac{2mm_{12}}{m+m_{12}}\,, \\ &V_{\rm cm}(X_{\rm cm}) = -2k\,X_{\rm cm}^2 + V(2X_{\rm cm}) = \begin{cases} +\infty & \text{for } X_{\rm cm} < 0 \\ 0 & \text{for } 0 < X_{\rm cm} < \frac{a}{2} \\ +\infty & \text{for } X_{\rm cm} > \frac{a}{2} \end{cases} \end{aligned} \tag{42}$$

$$H_{\rm rel} = \frac{P^2}{2m_{\rm rel}} + \frac{kX^2}{2}\,, \quad m_{\rm rel} = \frac{mm_{12}}{2(m_{12}-m)}\,, \tag{43}$$

The energy is positive if

$$m_{12} > m \tag{44}$$

(b) **13 marks.** Separate the variables and find the eigenvalues of the Hamiltonian for values of m_{12} and m from the previous question.

Answer. Since

$$H = H_{\rm cm} + H_{\rm rel}\,, \tag{45}$$

$X_{\rm cm}$ and X can be separated, and the eigenfunctions of H factorise

$$\psi_E(x_{\rm cm},x)=\psi_{E_{\rm cm}}(x_{\rm cm})\psi_{E_{\rm rel}}(x)\,,\quad E=E_{\rm cm}+E_{\rm rel} \tag{46}$$

where $\psi_{E_{\rm cm}}(x_{\rm cm})$ and $\psi_{E_{\rm rel}}(x)$ satisfy

$$\begin{gathered}\left(\frac{P_{\rm cm}^2}{2m_{\rm cm}}+V_{\rm cm}(X_{\rm cm})\right)\psi_{E_{\rm cm}}(x_{\rm cm})=E_{\rm cm}\psi_{E_{\rm cm}}(x_{\rm cm})\\ \left(\frac{P^2}{2m_{\rm rel}}+\frac{kX^2}{2}\right)\psi_{E_{\rm rel}}(x)=E_{\rm rel}\psi_{E_{\rm rel}}(x)\end{gathered} \tag{47}$$

The centre-of-mass Hamiltonian $H_{\rm cm}$ has the infinitely deep well potential. The wave functions and energy are

$$\psi_{E_{\rm cm}}(x_{\rm cm})=2\sqrt{\frac{1}{a}}\sin\frac{2\pi n_{\rm cm}x_{\rm cm}}{a}\,,\quad E_{\rm cm}=\frac{2\hbar^2\pi^2}{m_{\rm cm}a^2}n_{\rm cm}^2\,,\quad n_{\rm cm}=1,2,\dots \tag{48}$$

The relative-motion Hamiltonian $H_{\rm rel}$ is just a harmonic oscillator one with mass $m_{\rm rel}=\frac{mm_{12}}{2(m_{12}-m)}$ and frequency $\omega^2=k/m_{\rm rel}$. Thus,

$$E_{\rm rel}=\hbar\,\omega\,(n_{\rm rel}+\frac{1}{2})\,,\quad n_{\rm rel}=0,1,\dots \tag{49}$$

Thus, the total spectrum is

$$E=E_{\rm cm}+E_{\rm rel}=\frac{2\hbar^2\pi^2}{m_{\rm cm}a^2}n_{\rm cm}^2+\hbar\,\omega\,(n_{\rm rel}+\frac{1}{2}) \tag{50}$$

(c) **10 marks.** Find the normalised ground state wave function.

Answer. The ground state wave function is given by the product of

$$\psi_1(x_{\rm cm})=2\sqrt{\frac{1}{a}}\sin\frac{2\pi x_{\rm cm}}{a}\quad\text{for}\ \ 0<x_{\rm cm}<\frac{a}{2};\quad\psi_1(x_{\rm cm})=0\quad\text{for}\ \ x_{\rm cm}<0\ \text{and}\ x_{\rm cm}>\frac{a}{2} \tag{51}$$

and

$$\psi_0(x)=\frac{1}{\sqrt{\sqrt{2\pi}\eta_{\rm rel}}}\exp\big(-\frac{x^2}{4\eta_{\rm rel}^2}\big)\,,\quad\eta_{\rm rel}=\sqrt{\frac{\hbar}{2m_{\rm rel}\omega}} \tag{52}$$