

**PHASM426 / PHASG426**  
**Advanced Quantum Theory Problem Sheet 2**

Deadline: Tuesday 15th November 2016

Please hand in your completed work at the **end** of the lecture on that day. If you are unable to attend the lecture, you may scan your work, *save it as a single PDF file* and email it to me **prior** to this lecture. You may also bring the work to me in my office (B12) before the lecture. **Make sure your completed work is clearly labelled with your name and college.** Please note that UCL places severe penalties on late-submitted work.

1. Two quantum systems  $a$  and  $b$  are prepared in a joint state  $|\Psi\rangle = |\psi_a\rangle|\psi_b\rangle$ . Let the set  $\{|\phi_k\rangle\}$  be a basis of states for system  $a$ ,  $\{|\nu_j\rangle\}$  a basis for system  $b$  and  $A$  an operator on the Hilbert space of  $a$  with the following spectral decomposition:

$$A = \lambda_1|\phi_1\rangle\langle\phi_1| + \lambda_2 \sum_{n=2}^N |\phi_n\rangle\langle\phi_n|.$$

- (a) Write down an expression for the projector acting on the total Hilbert space and which is associated to the measurement outcome  $\lambda_2$ . Derive an expression for the probability of obtaining  $\lambda_2$  in a measurement of  $A$  on the state  $|\Psi\rangle$ .

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**Model answer:** Let's denote  $P_{\lambda_2}$  the projector associated to  $\lambda_2$ , then acting on the total Hilbert space this projector reads:

$$P_{\lambda_2} \otimes \mathbb{1}_b = \sum_{n=2}^N |\phi_n\rangle\langle\phi_n| \sum_j |\nu_j\rangle\langle\nu_j| = \sum_{n=2}^N \sum_j |\phi_n\rangle|\nu_j\rangle\langle\nu_j|\langle\phi_n|$$

Then the probability of obtaining  $\lambda_2 = \langle\Psi|P_{\lambda_2} \otimes \mathbb{1}_b|\Psi\rangle$  becomes:

$$\begin{aligned} \langle\Psi|P_{\lambda_2} \otimes \mathbb{1}_b|\Psi\rangle &= \sum_{n=2}^N \sum_j \langle\psi_a|\langle\psi_b||\phi_n\rangle|\nu_j\rangle\langle\nu_j|\langle\phi_n||\psi_a\rangle|\psi_b\rangle \\ &= \sum_{n=2}^N |\langle\psi_a|\phi_n\rangle|^2 \underbrace{\sum_j \langle\psi_b|\nu_j\rangle\langle\nu_j|\psi_b\rangle}_{=1} \\ &= \sum_{n=2}^N |\langle\psi_a|\phi_n\rangle|^2 \end{aligned}$$

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- (b) Derive an expression for the state  $|\Psi'\rangle$  of the global system after the measurement. Has the state of the system  $b$  changed?
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**Model answer:**

$$\begin{aligned} |\Psi'\rangle &= \frac{(P_{\lambda_2} \otimes \mathbb{1}_b)|\Psi\rangle}{\sqrt{\langle\Psi|P_{\lambda_2} \otimes \mathbb{1}_b|\Psi\rangle}} \\ &= \frac{\sum_{n=2}^N \langle\phi_n|\psi_a\rangle}{\sqrt{\sum_{n=2}^N |\langle\psi_a|\phi_n\rangle|^2}} |\phi_n\rangle|\psi_b\rangle = |\psi'_a\rangle|\psi_b\rangle. \end{aligned}$$


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- (c) Discuss whether the predictions in (a) and (b) would change depending of the choice of basis for the system  $b$ . Will the results of measurements on the systems  $a$  and  $b$  be correlated? Justify your answer.
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**Model answer:** The predictions in (a) and (b) would not change depending on the basis set for  $b$ . Also, if we find the probability of a particular eigenvalue of an operator acting on  $B$  the result will be analogous i.e. it will be independent on the basis set of  $a$ . This therefore means that measurement outcomes are uncorrelated.

[4]

**Marks** 2 marks for part (a). 1 mark for each part (b) and (c).

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2. In this question, we shall consider experiments which generates pure states probabilistically. Such a probability distribution over pure states can be represented by a (single) mixed state in the density matrix formalism. Write down a matrix representation for the density operator in each of the following three cases. You may express them in bra and ket notation or use a matrix representation, but in either case simplify your expressions as much as possible. Note that  $|\phi_1\rangle$ ,  $|\phi_2\rangle$  and  $|\phi_3\rangle$  are an orthonormal set of states.

- (a) The state  $|\phi_1\rangle$  is prepared with probability  $1/4$ , and the state  $(|\phi_1\rangle + i|\phi_2\rangle)/\sqrt{2}$  is prepared with probability  $3/4$ .

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*Model Answer:* The density matrix is:

$$\begin{aligned}
 \rho &= \frac{1}{4} |\phi_1\rangle\langle\phi_1| + \frac{3}{4} \frac{1}{2} (|\phi_1\rangle + i|\phi_2\rangle)(\langle\phi_1| - i\langle\phi_2|) \\
 &= \left(\frac{5}{8}\right) |\phi_1\rangle\langle\phi_1| + i \left(\frac{3}{8}\right) |\phi_2\rangle\langle\phi_1| - i \left(\frac{3}{8}\right) |\phi_1\rangle\langle\phi_2| + \left(\frac{3}{8}\right) |\phi_2\rangle\langle\phi_2| \\
 &= \frac{1}{8} \begin{bmatrix} 5 & -i3 \\ i3 & 3 \end{bmatrix}
 \end{aligned}$$


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(b) The following states are each prepared with probability  $1/3$ ,

- $(|\phi_1\rangle + |\phi_2\rangle)/\sqrt{2}$ ,
- $(|\phi_1\rangle + \exp(i2\pi/3)|\phi_2\rangle)/\sqrt{2}$ ,
- $(|\phi_1\rangle + \exp(-i2\pi/3)|\phi_2\rangle)/\sqrt{2}$ .

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*Model Answer:* The density matrix is:

$$\begin{aligned}
 \rho &= \frac{1}{3} \frac{1}{2} (|\phi_1\rangle + |\phi_2\rangle)(\langle\phi_1| + \langle\phi_2|) + \frac{1}{3} \frac{1}{2} (|\phi_1\rangle + \exp[i2\pi/3]|\phi_2\rangle)(\langle\phi_1| + \exp[-i2\pi/3]\langle\phi_2|) \\
 &\quad + \frac{1}{3} \frac{1}{2} (|\phi_1\rangle + \exp[-i2\pi/3]|\phi_2\rangle)(\langle\phi_1| + \exp[i2\pi/3]\langle\phi_2|) \\
 &= \left(\frac{1}{2}\right) (|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|) \\
 &= \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}
 \end{aligned}$$

[4]

**Marks.** Total marks are **4**, 2 marks for each part.

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3. The combined state of a pair of two-level atoms,  $A$  and  $B$ , is given by the density matrix:

$$\rho = \frac{1}{2} |g_A, g_B\rangle\langle g_A, g_B| + \frac{1}{2} |g_A, e_B\rangle\langle g_A, e_B|.$$

(a) Calculate the reduced density matrix operator for the each of the two-level systems.

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*Model answer:* Using  $\mathbb{1}_B = |g_B\rangle\langle g_B| + |e_B\rangle\langle e_B|$

$$\begin{aligned}
 \rho_A &= \text{Tr}_B(\rho \mathbb{1}_B) = \langle g_B | \rho | g_B \rangle + \langle g_B | \rho | e_B \rangle \\
 &= \frac{1}{2} |g_A\rangle\langle g_A| + \frac{1}{2} |g_A\rangle\langle g_A| = |g_A\rangle\langle g_A|.
 \end{aligned}$$

Similarly  $\rho_A = \text{Tr}_B(\rho \mathbb{1}_B) = \langle g_A | \rho | g_A \rangle + \langle e_A | \rho | e_A \rangle$  but in this case  $\langle e_A | \rho | e_A \rangle = 0$ . Then

$$\rho_A = \langle g_A | \rho | g_A \rangle = \frac{1}{2} |g_B\rangle \langle g_B| + \frac{1}{2} |e_B\rangle \langle e_B|.$$

$B$  is an statistical mixture of the ground and excited state.

- (b) Calculate the purity of system  $A$  and indicate whether the state of the two atoms is a product or an entangled state. Justify your answer.

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*Model answer:* The purity for a general state  $\rho$  is given by  $\text{Purity} = \text{Tr}(\rho^2)$ . Since  $\rho_A$  and  $\rho_B$  are diagonal in the basis chosen i.e.

$$\rho_A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \rho_B = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}.$$

the Purity is very simple to compute:  $\text{Tr}(\rho_A^2) = 1$  and therefore it cannot be in an entangled state with  $B$ . You can also notice that the joint state of  $A$  and  $B$ ,  $\rho$ , can be written as a mixed product state i.e.  $\rho = \rho_A \otimes \rho_B$ :

$$\rho = |g_A\rangle \langle g_A| \otimes \frac{1}{2} (|g_B\rangle \langle g_B| + |e_B\rangle \langle e_B|).$$

If we compute the purity of  $B$  we have  $\text{Tr}(\rho_B^2) = 1/2$ . Based alone of the purity of  $B$  we cannot conclude anything about the entanglement between  $A$  and  $B$ .

[3]

**Marks:** Total marks is 3. 2 for part (a) and 1 for part (b).

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4. A physicist runs two experiments  $A$  and  $B$  to prepare quantum systems in a variety of initial states. In experiment  $A$  she uses a probabilistic machine that can prepare a single quantum system in one of  $n$  possible pure states  $\{|\Psi_1\rangle, |\Psi_2\rangle, \dots, |\Psi_n\rangle\}$  with corresponding probabilities  $\{p_1, p_2, \dots, p_n\}$ . In experiment  $B$ , instead, she generates  $m$  non-interacting quantum systems, each of them prepared in its corresponding lower energy state  $\{|\Phi_1\rangle, |\Phi_2\rangle, \dots, |\Phi_m\rangle\}$ . Let  $\rho_A$  and  $\rho_B$  be the density matrix operators for the quantum states prepared in experiments  $A$  and  $B$ , respectively.

- (a) Let  $P_j$  and  $P_k$  be the projectors associated to the states  $|\Psi_j\rangle$  and  $|\Psi_k\rangle$  produced by  $A$ . Discuss whether the product  $P_j P_k$  vanishes. Justify your answer.

[1]

*Model answer:*  $P_j P_k = |\Psi_j\rangle \langle \Psi_j| |\Psi_k\rangle \langle \Psi_k|$ . Since the states  $|\Psi_j\rangle$  and  $|\Psi_k\rangle$  are in general not orthogonal, then  $\langle \Psi_j | \Psi_k \rangle \neq 0$  in general. Hence  $P_j P_k$  does not vanish in general.

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- (b) Derive expressions for  $\rho_A$  and  $\rho_B$  and justify your answers in detail. [3]

*Model answer:* In experiment A the physicist is generating an statistical mixture of quantum states, hence

$$\rho_A = \sum_{j=1}^n p_j |\Psi_j\rangle \langle \Psi_j|.$$

In experiment B the physicist is generating non interacting systems, each of them in a specific pure quantum state, hence

$$\rho_B = |\Phi_1\rangle \langle \Phi_1| \otimes |\Phi_2\rangle \langle \Phi_2| \otimes \cdots \otimes |\Phi_m\rangle \langle \Phi_m|.$$

*Marks:* 1 for each correct density matrix operator and 1 for justification.

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- (c) Let  $O_A$  be a Hermitian operator describing an observable of the system produced by  $A$ . Derive an expression for the expected value of  $O_A$ . [1]

*Model answer:*

$$\langle O_A \rangle = \text{Tr}[\rho_A O_A] = \sum_{j=1}^n p_j \langle \Psi_j | O_A | \Psi_j \rangle.$$

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- (d) Let  $O_B^k$  be a Hermitian operator describing an observable of the  $k$ th system produced by  $B$ . Derive an expression for the expected value of  $O_B^k$ . [1]

*Model answer:*

$$\langle O_B^k \rangle = \langle \Phi_k | O_A | \Phi_k \rangle.$$

Justification: the reduced state of the  $k$ th system is  $\rho_k = |\Phi_k\rangle \langle \Phi_k|$  i.e. sytem  $k$  is in a pure state.

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5. Similar to the position basis, we can consider the continuous momentum basis  $|p\rangle$ . This is a Dirac delta-normalised basis which represents eigenstates of the momentum operator,  $\hat{p}|p\rangle = p|p\rangle$ , where the eigenvalues  $p$  take any real value. The closure relationship  $\mathbb{1} = \int_{-\infty}^{\infty} dp |p\rangle \langle p|$  is satisfied. One can show that the momentum basis states satisfy the following inner product with respect to the position basis:

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

In analogy to the position wave-function, we can define a momentum wave-function,  $\Psi(p) = \langle p|\psi\rangle$ . Show that  $\Psi(p)$  is the Fourier transform of the position wave-function  $\psi(x)$ , i.e.

$$\Psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) dx$$

[2]

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*Model answer*

$$\begin{aligned} \Psi(p) &= \langle p| \left( \int_{-\infty}^{\infty} dx |x\rangle \langle x| \right) |\psi\rangle = \int_{-\infty}^{\infty} dx \langle p|x\rangle \langle x|\psi\rangle \\ &= \int_{-\infty}^{\infty} dx (\langle x|p\rangle)^* \psi(x) = \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \psi(x) \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ipx/\hbar} \psi(x) = \mathcal{F}[\psi(x)] \end{aligned}$$

**Marks.** 2 Marks for complete derivation. Partial marks for partial answer.

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6. In this question we will explore why we can neglect term  $S_2(x)$  in the expansion of  $S(x)$  in the derivation of the WKB wavefunction, when the potential  $V(x)$  is slowly varying with respect to the local de Broglie wavelength.

In the lectures we showed that the TISE may be written, using the Ansatz  $\psi(x) = \exp[iS(x)]$  as:

$$-\frac{i\hbar}{2m} S''(x) + \frac{1}{2m} S'(x)^2 + V(x) - E = 0.$$

where  $'$  denotes the derivative with respect to  $x$ , and  $''$  the second derivative with respect to  $x$ .

We then replaced  $S(x)$  with the series expansion  $S(x) = \sum_j \hbar^j S_j(x)$  and derived zeroth and first order equations from which we derived expressions:

$$S'_0(x) = p(x) \quad S_1(x) = \frac{i}{2} \log p(x)$$

where for simplicity I have neglected the  $\pm$  signs.

- (a) By considering terms in the above equation proportional to  $\hbar^2$  derive the second order equation:

$$S'_2(x) = \frac{iS''_1(x) - S'_1(x)^2}{2S'_0(x)}$$

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*Model answer:* We consider only the terms in our rewritten TISE which are to the second order in  $\hbar$ , e.g. proportional to  $\hbar^2$ . This gives us:

$$-\frac{i\hbar}{2m}\hbar S_1''(x) + \frac{1}{2m}\hbar^2(S_1'(x)^2 + 2S_0'(x)S_2'(x)) = 0.$$

We cancel the  $\hbar^2$  and  $2m$  factors and rearrange to achieve the above expression.

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(b) Using the definitions for  $S_0'(x)$  and  $S_1(x)$  above show that:

$$S_2'(x) = \frac{1}{8} \left( \frac{3p'(x)^2}{p(x)^3} - \frac{2p''(x)}{p(x)^2} \right)$$


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We need to compute  $S_1'(x)$  and  $S_1''(x)$ .

$$S_1'(x) = \frac{i}{2} \frac{p'(x)}{p(x)}$$

via the chain rule. Using the product rule or quotient rule, we achieve:

$$S_1''(x) = \frac{i}{2} \left[ \frac{p''(x)}{p(x)} - \frac{p'(x)^2}{p(x)^2} \right]$$

and substituting this into the expression derived in 1(a) recovers the correct expression.

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(c) And verify that the following expression is a solution to this differential equation:

$$S_2(x) = -\frac{1}{4} \frac{p'(x)}{p(x)^2} - \frac{1}{8} \int^x \frac{p'(y)^2}{p(y)^3} dy,$$

where  $y$  is a dummy integration variable.

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To verify, we differentiate this expression once:

$$S_2'(x) = -\frac{1}{4} \left[ \frac{p''(x)}{p(x)^2} - 2 \frac{p'(x)^2}{p(x)^3} \right] - \frac{1}{8} \frac{p'(x)^2}{p(x)^3}.$$

using the product or quotient rules and the fundamental theorem of calculus. Simplifying we verify that the expression is indeed a solution to the above differential equation.

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- (d) To be able to neglect the term containing  $S_2(x)$  in the series expansion for  $S(x)$  we need that  $|\hbar S_2(x)| \ll 1$ . We will focus solely on the first term in  $S_2(x)$  (a similar analysis can be performed on the second term, but is more complicated due to the integral). If the local de Broglie wavelength is defined  $\lambda(x) = h/p(x)$  show that

$$\left| \hbar \frac{p'(x)}{p(x)^2} \right| \ll 1$$

implies

$$\left| \frac{1}{2\pi} \lambda'(x) \right| \ll 1.$$

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We differentiate  $\lambda(x)$ :

$$\lambda'(x) = -\frac{hp'(x)}{p(x)^2}$$

and substitute it into the first inequality. Upon cancelling the  $h$  factor we achieve the second inequality.

[4]

**Marks:** total marks are **4**. 1 mark for each numeral and partial marks for partial answers.

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7. Consider a particle of mass  $m$  in a potential such that  $V(x) = 0$  for  $|x| > \kappa$  and  $V(x) = -V_0 \left(1 - \frac{|x|}{\kappa}\right)$  for  $|x| \leq \kappa$ . Given that  $mV_0\kappa^2/\hbar^2 = 18$  calculate the number of bound states and their energies expressed in terms of  $V_0$ .

You may use the integral

$$\int (1-y)^{1/2} dy = \frac{-2}{3} (1-y)^{3/2} + c$$

and use the WKB quantisation condition for a smooth well derived in lectures:

$$\int_a^b p(x') dx' / \hbar = \left(n + \frac{1}{2}\right) \pi$$

where  $a$  and  $b$  are the positions of the classical turning points on the left and right of the well, respectively, and  $x'$  is a dummy integration variable ( $x'$  does not mean  $dx/dx$ ).

Hint: By sketching the form of the potential, consider whether the energy of a bound particle will be positive or negative. Think about how the energy of the



particle affects the classical turning points in this problem, and how that affects, in turn, the integral in the quantisation condition.

[3]

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*Model answer:* We use the WKB quantisation condition derived in lectures:

$$\int_a^b p(x') dx' = \left(n + \frac{1}{2}\right) \hbar \pi$$

where  $p(x) = \sqrt{2m(E - V(x))}$ . To use this, we need to identify the positions of the classical turning points  $a$  and  $b$ , where  $E = V(x)$ . Since the potential is symmetric around  $x = 0$ , the turning points will be at  $a = -|T|$  and  $b = +|T|$ . We solve  $E = V(x)$  to find the classical turning point as a function of energy.

$$E = -V_0 \left(1 - \frac{T}{\kappa}\right)$$

Hence

$$T = \kappa \left(1 + \frac{E}{V_0}\right) = \kappa \frac{E + V_0}{V_0}$$

The WKB quantisation condition can thus be written

$$\begin{aligned} \int_{-T}^T p(x') dx' &= \left(n + \frac{1}{2}\right) \hbar \pi \\ &= \int_{-T}^T \left(2m \left(E + V_0 \left(1 - \frac{|x'|}{\kappa}\right)\right)\right)^{1/2} dx' \\ &= 2\sqrt{2m} \int_0^T \left((E + V_0) - \frac{x' V_0}{\kappa}\right)^{1/2} dx' \\ &= 2\sqrt{2m(E + V_0)} \int_0^T \left(1 - \frac{x' V_0}{\kappa(E + V_0)}\right)^{1/2} dx' \\ &= 2\sqrt{2m(E + V_0)} \int_0^T \left(1 - \frac{x'}{T}\right)^{1/2} dx' \end{aligned}$$

where we identified the expression for  $1/T$  within the integral. Using the substitution  $y = x'/T$  and integrating using the standard integral above, we obtain

$$\frac{4}{3} \sqrt{2m} \frac{\kappa(E + V_0)^{3/2}}{V_0} = \left(n + \frac{1}{2}\right) \hbar \pi$$

which we can write

$$\frac{4}{3} \sqrt{2} \sqrt{\frac{m \kappa^2 V_0}{\hbar^2}} \left(\frac{E + V_0}{V_0}\right)^{3/2} = \left(n + \frac{1}{2}\right) \pi$$

we now substitute in the condition  $mV_0\kappa^2/\hbar^2 = 18$  to obtain

$$\frac{4}{3}\sqrt{36}\left(\frac{E+V_0}{V_0}\right)^{3/2} = \left(n + \frac{1}{2}\right)\pi$$

which we rewrite to obtain an expression for the quantised energies  $E$

$$E = -V_0 + V_0 \left( \frac{1}{8} \left( n + \frac{1}{2} \right) \pi \right)^{2/3}$$

For this potential, bound states must have energies  $E < 0$  (indeed our WKB treatment only holds in this region, since otherwise there is no classical turning point) implying

$$\left( \frac{1}{8} \left( n + \frac{1}{2} \right) \pi \right)^{2/3} < 1$$

which give  $n < 2.046$ . There are therefore **3 bound states**  $n = 0, 1$  and  $2$ . Substituting in these values, we obtain the three energy values  $E/V_0 = -0.66, -0.30, -0.01$ .

**Marks:** Total marks are **3**. **1 mark** for correctly identifying the classical turning points and for successfully integrating the WKB quantisation integral (partial mark for partial success). **1 mark** for correctly substituting in  $mV_0\kappa^2/\hbar^2 = 18$  and for recognising that bound states need  $E < 0$  for this potential. **1 mark** for identifying  $n < 2.046$  and concluding that this leads to 3 bound states and correctly calculating their energies.