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Quantum Mechanics I
1st Midterm Exam

9th Oct. '98.
Solutions (T. Hübsch)

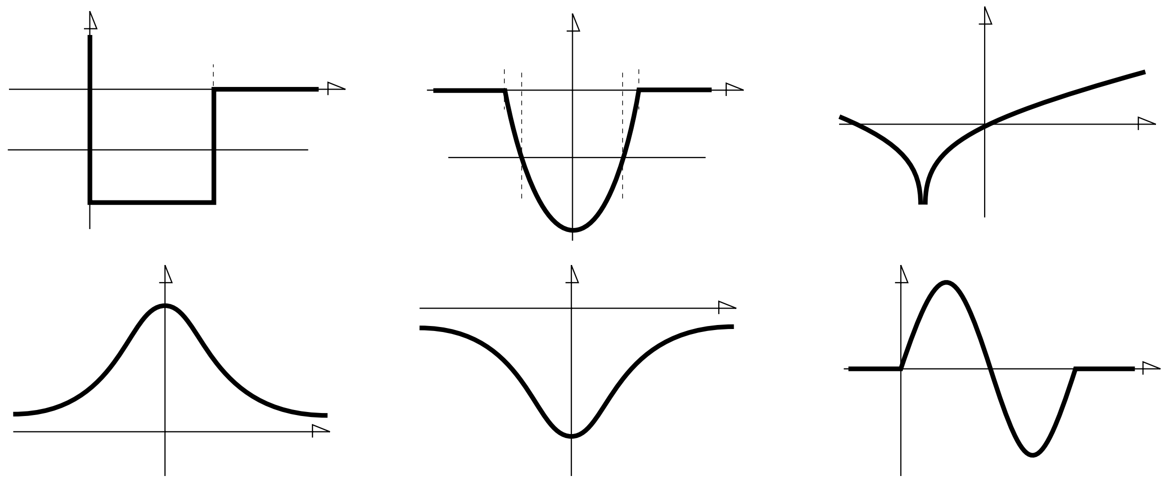

Figure 1. A sketch of the potentials in problems 1, 2, and 4.a–4.d.

1.a: As in all piece-wise constant potential problems, we divide the domain of x into two regions, according to whether $E > V(x)$ or $E < V(x)$. Note that it is unnecessary to consider $x < 0$, as the potential is infinitely strong there and the wave function must vanish. The first region is then $0 < x < a$, where $E < V(x)$, which is where we expect an oscillatory solution. The solutions in the second region ($a < x < \infty$) is exponentially decaying, and in addition. Therefore, we can write

$$\psi_1 = A\sin(kx+\delta) \ , \qquad \psi_2 = Be^{-\kappa x} \ , \tag{1}$$

where $\hbar\kappa = \sqrt{2m|E|}$, $\hbar k = \sqrt{2m(E+V_0)}$. The matching conditions are: $\psi_1(0)$=0 which implies δ=0, $\psi_1(a)$=$\psi_2(a)$ and $\psi_1'(a)$=$\psi_2'(a)$.

1.b: The wave-function in the first region has been chosen so as to most effectively find the energy quantization condition—as discussed in class. In calculating the logarithmic derivative, a single function like $\sin(kx)$ is preferable to a linear combination of two exponentials. We calculate $\frac{1}{\psi}\frac{\mathrm{d}\psi}{\mathrm{d}x}$ for each of ψ_1, ψ_2 and impose the matching across the two boundary at $x = a$ of the logarithmic derivative:

$$\frac{1}{\psi_1}\frac{\mathrm{d}\psi_1}{\mathrm{d}x}\Big|_{x=-a} = k\cot[k(-a)] = -k\cot(ka) \ \stackrel{!}{=}\ \frac{1}{\psi_2}\frac{\mathrm{d}\psi_2}{\mathrm{d}x}\Big|_{x=-a} = \kappa \ . \tag{2}$$

Therefore

$$n\pi - \arctan\Big(\frac{k}{\kappa}\Big) = ka \ , \tag{3}$$

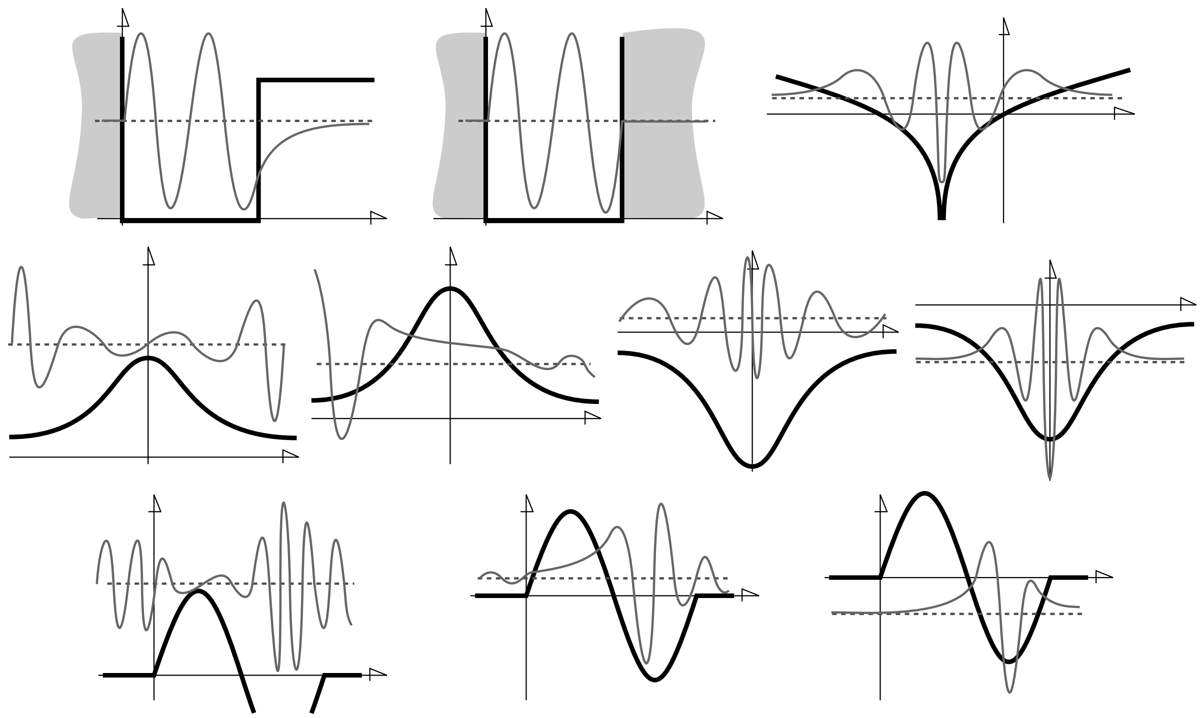

Figure 2. A sketch of a sample wave function for problems: 1.a and 1.c with the energy level as given, and 4.a–d for all possible energy levels. The choice of (a)symmetry of the wave functions was random.

The $n\pi$ must be included because of the periodicity of arctan. This then is the relation which determines E; nothing more, nothing less. One can merely make it more explicit by substituting the expressions for k and κ:

$$n\pi - \arctan\Big(\sqrt{\frac{V_0+E}{|E|}}\Big) = \frac{a}{\hbar}\sqrt{2m(V_0+E)}\ . \tag{4}$$

1.c: The limit $V_0 \to \infty$ has been discussed in class: the $V_0 \to \infty$ limit then simply reproduces the infinite potential well, where the wave function must vanish at both 'walls', at 0 and at a; there are no conditions on the derivatives of the wave functions.

1.d: The wave function can be written as $\psi = A\sin(kx)$, ensuring that $\psi(0) = 0$. The other boundary condition, $\psi(a) = 0$ then sets $k_n = n\pi/a$. This then produces the energy quantization condition

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}\ . \tag{5}$$

The ground state being ψ_1, $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$ is the energy of the ground state.

Note that the result (5) could have been obtained from (3) through a careful evaluation of the limits: Upon shifting as described in part c., E now being positive, we have

$$n\pi - \arctan\Big(\sqrt{\frac{V_0+E}{|E|}}\Big) = \frac{a}{\hbar}\sqrt{2m(V_0+E)}\ . \tag{6}$$

In the limit $V_0 \to +\infty$, $\sqrt{\frac{E}{V_0 - E}} \to 0$, and since $\arctan 0 = 0$, the result (5) follows.

2.a: Before we deal with parts a. and b., note that only the energies $E > -\lambda a^2$ are allowed: states with energies below that would diverge and so be utterly unnormalizable.

For negative energies, $-\lambda a^2 < E < 0$, only the region between the classical turning points, $\pm b$, is allowed. These turning points occur where $E{=}V(\pm b)$, and so $b = \sqrt{a^2 - |E|/\lambda}$; clearly, $0 < b < a$.

Let us write

$$\hbar k(x) \stackrel{\text{def}}{=} \sqrt{2m\big(E - \lambda(x^2 - a^2)\big)}\ , \quad \hbar\kappa(x) \stackrel{\text{def}}{=} \sqrt{2m\big(\lambda(x^2 - a^2) - E\big)}\ . \tag{7}$$

The WKB solutions are either

$$\psi(x) = \frac{A}{\sqrt{k(x)}}\ e^{i\int_c^x \mathrm{d}x\, k(x)} + \frac{B}{\sqrt{k(x)}}\ e^{-i\int_c^x \mathrm{d}x\, k(x)}\ , \tag{8}$$

for the classically allowed region, or

$$\psi(x) = \frac{C}{\sqrt{\kappa(x)}}\ e^{-\int_c^x \mathrm{d}x\, \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\ e^{+\int_c^x \mathrm{d}x\, \kappa(x)}\ , \tag{9}$$

for the classically forbidden region, where c denotes the left hand side turning point, to be replaced by $-b$ and $+b$, as appropriate—closely following the case examined on p.108–109.

For $x < -b$ we have

$$\psi_1(x) = \frac{C}{\sqrt{\kappa(x)}}\ e^{-\int_{-b}^x \mathrm{d}x\, \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\ e^{+\int_{-b}^x \mathrm{d}x\, \kappa(x)}\ . \tag{10}$$

Notice that in these integrals, the lower limit is to the right of the upper one! Thus, for $x < -b$, these integrals are negative, so the first term diverges towards large and *negative* x, while the second term decays there. The boundary condition $\lim_{x\to-\infty} \psi(x) = 0$ then forces us to set $C = 0$.

In the region $-b < x < +b$, the WKB solution becomes

$$\begin{aligned}\psi_2(x) &= \frac{A}{\sqrt{k(x)}}\ e^{+i\int_{-b}^x \mathrm{d}x\, k(x)} + \frac{B}{\sqrt{k(x)}}\ e^{-i\int_{-b}^x \mathrm{d}x\, k(x)}\ ,\\ &= \frac{Ae^{+i\phi}}{\sqrt{k(x)}}\ e^{+i\int_{+b}^x \mathrm{d}x\, k(x)} + \frac{Be^{-i\phi}}{\sqrt{k(x)}}\ e^{-i\int_{+b}^x \mathrm{d}x\, k(x)}\ ,\end{aligned} \tag{11}$$

where

$$\phi \stackrel{\text{def}}{=} \int_{-b}^{+b} \mathrm{d}x\, k(x)\ . \tag{12}$$

The two constants A, B are determined in terms of C, D above through the WKB matching conditions, Eqs. (4.52a,b) in Park.

Finally, in the third region $x > +b$, the WKB solution takes the form

$$\psi_3(x) = \frac{C'}{\sqrt{\kappa(x)}}\ e^{-\int_b^x \mathrm{d}x\, \kappa(x)} + \frac{D'}{\sqrt{\kappa(x)}}\ e^{+\int_b^x \mathrm{d}x\, \kappa(x)}\ , \tag{13}$$

where C', D' are determined from A, B using Park's Eq. $(4.51a, b)$. This produces (using that $C = 0$):

$$\begin{aligned}C' &= \tfrac{1}{2}\big(\vartheta^*(Ae^{+i\phi}) + \vartheta(Be^{-i\phi})\big) = \tfrac{1}{2}\big(\vartheta^*(\vartheta^* De^{+i\phi}) + \vartheta(\vartheta De^{-i\phi})\big) \;, \\ &= \tfrac{1}{2i}(e^{+i\phi} - e^{-i\phi})D = D\sin\phi \;; \qquad (14a) \\ D' &= \vartheta(Ae^{+i\phi}) + \vartheta^*(Be^{-i\phi}) = \vartheta(\vartheta^* De^{+i\phi}) + \vartheta^*(\vartheta De^{-i\phi}) \;, \\ &= (e^{+i\phi} + e^{-i\phi})D = 2D\cos\phi \;. \qquad (14b)\end{aligned}$$

since $\vartheta^2 = i$ and $(\vartheta^*)^2 = -i$—just as given in the display preceding Eq. $(4.55a)$. The complete derivation here is included for the Students' benefit; it was not required in the test. Quoting the correct equations from the text sufficed.

It now remains to enforce the last boundary condition, $\lim_{x\to\infty}\psi(x) = 0$.

2.b: The boundary condition $\lim_{x\to\infty}\psi(x) = 0$ forces us to set $D' = 0$ (as this is now the term that diverges for large and *positive* x). Since $D' = D\cos\phi$ and $D \neq 0$ (or else the whole wave functions vanishes trivially), we must require that $\phi = (n+\frac{1}{2})\pi$.

Now as to the integral:

$$\begin{aligned}\phi &= \int_{-b}^{+b} \mathrm{d}x\, k(x) = \frac{\sqrt{2m}}{\hbar}\int_{-b}^{b} \mathrm{d}x\, \sqrt{E - \lambda(x^2 - a^2)} \;, \qquad (15a) \\ &= \frac{\sqrt{2m\lambda}}{\hbar} 2\int_0^b \mathrm{d}x\, \sqrt{b^2 - x^2} = \frac{\sqrt{2m\lambda}}{\hbar} 2b^2 \int_0^1 \mathrm{d}\xi\, \sqrt{1-\xi^2} \;, \qquad (15b)\end{aligned}$$

where between the first and the second row we used that $E = \lambda(b^2 - a^2)$, and then introduced the dimensionless variable $\xi = x/b$. The advantage of these modifications is in obtaining a result with a purely numerical integral; that is, the value of the as yet uncalculated integral is a dimensionless number—all the dependence on the observables has already been made explicit. The integral itself is not difficult:

$$\int \mathrm{d}\xi\, \sqrt{1-\xi^2} = \tfrac{1}{2}\xi\sqrt{1-\xi^2} + \tfrac{1}{2}\arcsin(\xi) \;, \qquad \int_0^1 \mathrm{d}\xi\, \sqrt{1-\xi^2} = \frac{\pi}{4} \;.$$

Thus,

$$(n+\tfrac{1}{2})\pi \stackrel{!}{=} \phi = \frac{\sqrt{2m\lambda}}{\hbar} 2\Big(a^2 + \frac{E_n}{\lambda}\Big)\frac{\pi}{4} \;, \qquad (16)$$

or,

$$E_n = \sqrt{\frac{2\lambda}{m}}(n+\tfrac{1}{2}) - \lambda a^2 \;. \qquad (17)$$

Notice that this makes perfect sense: within $-b < x < b$, the potential is that of the linear harmonic oscillator with the frequency $\sqrt{2\lambda/m}$, with the minimum of the potential being at $-\lambda a^2$ rather than at zero.

3. Following the hint, finding the *asymptotic* form of the wave function for $x \to \infty$ implies solving the Schrödinger equation approximately, working to highest order in x. So, our case being $k = 4$, we consider

$$\psi'' - \frac{2m}{\hbar^2}[\lambda x^{2k} - E]\psi = 0 \;, \qquad k \geq 1 \;, \qquad (18)$$

E may be neglected compared to $V(x)$ when x is large.

as in class, we calculate

$$\psi_\infty(x) = e^{-\alpha x^\beta}, \qquad \alpha, \beta \text{ constants}, \tag{19a}$$

$$\psi'_\infty(x) = -\alpha\,\beta\,x^{\beta-1}\,e^{-\alpha x^\beta}, \tag{19b}$$

$$\begin{aligned}\psi''_\infty(x) &= \big((-\alpha\,\beta\,x^{\beta-1})^2 - \alpha\,\beta(\beta-1)x^{\beta-2}\big)\,e^{-\alpha x^\beta}, \\ &= \big(\alpha^2\beta^2x^{2\beta-2} - \alpha\,\beta(\beta-1)x^{\beta-2}\big)\,e^{-\alpha x^\beta}, \\ &\approx (\alpha^2 m^2 x^{2\beta-2})\,e^{-\alpha x^\beta}, \qquad x\to\infty, \quad m>0\,.\end{aligned} \tag{19c}$$

The Schrödinger equation then implies (to highest order in x):

$$(\alpha\beta)^2\,x^{2\beta-2}\,e^{-\alpha x^\beta} \approx \frac{2m}{\hbar^2}\lambda x^{2k}\,e^{-\alpha x^\beta}\,. \tag{20}$$

For this to hold for any x, both the powers and the coefficients must be set equal, whence $m = k{+}1$ and then $\alpha = \sqrt{2m\lambda}/(\beta\hbar) = \sqrt{2m\lambda}/[(k{+}1)\hbar]$, and so finally

$$\psi(x) \approx \exp\big\{-\tfrac{\sqrt{2m\lambda}}{(k+1)\hbar}x^{k+1}\big\}, \quad \text{or,} \quad \psi(x) \approx e^{-\frac{\sqrt{2m\lambda}}{5\hbar}x^5}. \tag{21}$$

4.a: Firstly, note that the potential diverges (approaches $-\infty$) when $x\to-1$; thus, the minimum of $V(x)$ is $-\infty$, is at $x=-1$ and there is no lower bound for E. Furthermore, the potential $V(x) = V_0\log|x{+}1|$ grows unboundedly for both $x\to\pm\infty$. Thus, no matter how high an energy level, E, we choose, for some sufficiently negative or sufficiently positive x, the potential function will be bigger than E. Therefore, there are only bound (localized) states for this potential, and all energies are discrete (quantized); see Fig. 2. WKB provides a good estimate for the energy levels:

$$(n{+}\tfrac{1}{2})\pi \stackrel{!}{=} \frac{\sqrt{2m}}{\hbar}\int_a^b \mathrm{d}x\,\sqrt{E_n - V_0\log|x+1|}\,, \tag{22}$$

where $a = -(1+e^{E/V_0})$ and $b = 1 - e^{E/V_0}$. Amusingly, the integral in fact does have an exact solution (dividing the range into two parts, $x<-1$ and $x>-1$, and using:

$$\int \mathrm{d}\xi\,\sqrt{E_n - V_0\log\xi} = \xi\sqrt{E_n - V_0\log\xi} + \tfrac{1}{2}e^{E_n/V_0}\sqrt{\pi V_0}\big[1 + \mathrm{Erf}\big(\tfrac{E_n}{V_0} - \log\xi\big)\big]\,. \tag{23}$$

4.b: The potential $V(x) = V_0/(1{+}x^2)$ approaches zero at both $x\to\pm\infty$, and which is also the minimum of $V(x)$. Thus, the energies, E are bounded from below, by zero; that is, $E\geq 0$. At the same time, since the potential vanishes at both 'ends', no boundary conditions are obtained for either of $x\to\pm\infty$, and none of the stationary states are bound: they are all oscillatory; see Fig. 2.

4.c: The potential $V(x) = -V_0/(1{+}x^2)$ has its minimum at $V(0) = -V_0$. Thus the energy is bounded from below, by $-V_0$; that is, $E > -V_0$. The limit of $V(x)$ at either $x\to\pm\infty$ is zero. Thus, for $E>0$, there is no boundary condition on the stationary states at either of $x \to \pm\infty$, and these states are 'scattering' states, and E is continuous. However, for $-V_0 < E < 0$, for sufficiently negative and for sufficiently positive values of x, the energy E is less than the potential, and the wave functions must decay towards $x \to \pm\infty$. These are the bound states. The turning points are at $b = \pm\sqrt{V_0/|E| - 1}$. Again, we use WKB to obtain an estimate:

$$(n+\tfrac{1}{2})\pi \stackrel{!}{=} \frac{\sqrt{2m}}{\hbar}\int_{-b}^{b} \mathrm{d}x\ \sqrt{E_n - V_0/(1+x^2)}\ , \tag{24}$$

which is a fairly complicated, but still soluble integral.

4.d: The potential $V(x) = 0$ for $x < 0$ and $x > 2a$, but $V(x) = V_0 \sin(x\pi/a)$ offers the most diversity. Its minimum is $\min[V(x)] = -V_0$, at $x = 3a/2$, and its limits at either $x \to \pm\infty$ are $\lim_{x\to\pm\infty} V(x) = 0$. Thus, the energies are bounded from below by $-V_0$. On the other hand, for $E > 0$, there can be no boundary conditions on the wave functions (whose energies are now bigger than the potential at either of $x \to \pm\infty$), and these are the 'scattering' states, with continuous energies, E. So, the bound states are found only for $-V_0 < E < 0$, when the energy is less than the potential as $x \to \pm\infty$. Again, we can use WKB to estimate the energy levels:

$$(n+1)\pi \stackrel{!}{=} \frac{\sqrt{2m}}{\hbar}\int_{b_1}^{b_2} \mathrm{d}x\ \sqrt{E_n - V_0\sin(x\pi/a)}\ , \tag{25}$$

where the turning points, $0 < b_1, b_2 < 2a$ are the two solutions of $E = V_0\sin(x\pi/a)$.