Midterm II Solutions

TA: Kate Storey-Fisher
Prof: Javad Shabani
Quantum Mechanics 1
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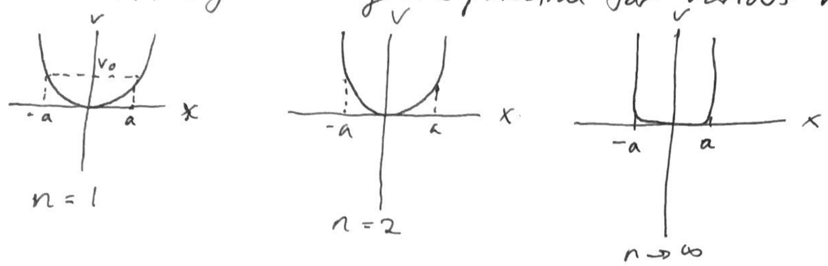
1. 1D Potential: $V(x) = V_0\left(\frac{x}{a}\right)^{2n}$, mass μ

Let's start by sketching the potential for various n:



For $n=1$, it becomes exactly a harmonic oscillator (HO), with $\frac{1}{2}\mu\omega^2 = \frac{V_0}{a^2}$.
For $n\to\infty$, it approaches an infinite square well. (ISW)

Energy eigenvalue distribution: An HO has evenly spaced (linearly) energy levels, $E_n \propto n$, and an ISW has quadratically spaced levels, $E_n \propto n^2$. So as the n in our $V(x)$ increases (note: diff n than energy levels!), we should expect the spacings between levels to increase from linear to quadratic.

Parity: The potential is always even, so the wavefunctions will always have definite parity, specifically alternating between even and odd.

We can use the uncertainty principle to estimate the ground state energy, because we expect that the ~~...~~ position p should be greater than the spread in position Δx, and the momentum p should be greater than the spread in momentum Δp. So the energy is:

$$E = T + V = \frac{p^2}{2\mu} + V_0\left(\frac{x}{a}\right)^{2n} \Rightarrow E \geq \frac{(\Delta p)^2}{2\mu} + V_0\left(\frac{\Delta x}{a}\right)^{2n} = E_0 \rightarrow \text{GS energy is lowest energy}$$

From the uncertainty principle $\Delta x \Delta p \sim \frac{\hbar}{2} \Rightarrow \Delta p \sim \frac{\hbar}{2\Delta x}$, so

$$E_0 = \frac{1}{2\mu}\left(\frac{\hbar}{2\Delta x}\right)^2 + V_0\left(\frac{\Delta x}{a}\right)^{2n} = \frac{\hbar^2}{8\mu}(\Delta x)^{-2} + \frac{V_0}{a^{2n}}(\Delta x)^{2n}$$

Let's find the Δx that minimizes this:

$$\frac{dE_0}{d(\Delta x)} = \frac{\hbar^2}{8\mu}(-2)(\Delta x)^{-3} + 2n\frac{V_0}{a^{2n}}(\Delta x)^{2n-1} = 0 \xrightarrow{\text{solve}} \Delta x = \left(\frac{\hbar^2 a^{2n}}{8\mu V_0 n}\right)^{\frac{1}{2n+2}}$$

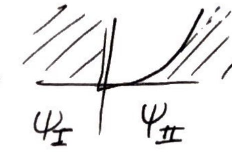
plug back in $\Rightarrow$
$$\boxed{E = \frac{\hbar^2}{8\mu}\left(\frac{\hbar^2 a^{2n}}{8\mu V_0 n}\right)^{\frac{-1}{n+1}} + \frac{V_0}{a^{2n}}\left(\frac{\hbar^2 a^{2n}}{8\mu V_0 n}\right)^{\frac{n}{n+1}}}$$

For $n=1$, find that $E = \frac{\hbar}{a}\sqrt{\frac{V_0}{2\mu}}$. To relate to HO formulation, $\frac{1}{2}\mu\omega^2 = \frac{V_0}{a^2}$, plug in $\Rightarrow \boxed{E = \frac{1}{2}\hbar\omega}$ as expected for HO!

For $n\to\infty$, first term $\to 0$, second term $\to V_0 a^{-\frac{2n}{n+1}}\left(\frac{\hbar^2}{8\mu V_0}\right)^{\frac{n}{n+1}} n^{-\frac{n}{n+1}} \Rightarrow \boxed{E = \frac{\hbar^2}{8\mu a^2}}$.

This is very close to the ISW with width $2a$, $E_0 = \frac{\hbar^2\pi^2}{2\mu(2a)^2}$; off by a factor of π^2

2. Half harmonic oscillator, $V = \begin{cases} \frac{1}{2}m\omega^2x^2 & x \geq 0 \\ \infty & x \leq 0 \end{cases}$



a) We can keep the same form of solutions as the full harmonic oscillator,

$$\psi_n(x) = A_n H_n(\xi)\, e^{-\xi^2/2},$$

but with the added boundary condition $\psi(0) = 0$.

The Hermite polynomials are defined as $H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$, and we can see that the even n's will have a constant term ($H_0(x) = 1$, $H_2(x) = x^2 - 1, \dots$) and the odd terms will all be polynomials with higher order of x ($H_1(x) = x$, $H_3(x) = x^3 - 3x, \dots$).

So only the odd terms satisfy the BC, so the possible energies are:

$$\boxed{E = (n + \tfrac{1}{2})\hbar\omega \text{ with } n = 1, 3, 5, \dots \quad \text{OR} \quad E = (2n - \tfrac{1}{2})\hbar\omega,\ n = 1, 2, 3 \dots}$$

You can also show this by going back to the analytic method and see that $a_0 = 0$ to satisfy the BC, killing all even terms from the beginning.

b) We know the original groundstate wave function is already normalized for us, so we can use the fact that we are now restricted to half the space to normalize it with fewer gross integrals (note that this ground state corresponds to orig ψ_1):

$$1 = A^2 \int_0^\infty |\psi_{GS}|^2 = A^2 \Big(\frac{1}{2} \underbrace{\int_{-\infty}^{\infty} |\psi_1|^2}_{1} \Big) = \frac{1}{2} A^2 \Rightarrow A^2 = 2 \Rightarrow A = \sqrt{2}$$

$$\Rightarrow \boxed{\psi_{GS} = \sqrt{2}\,\psi_{1,\text{orig}} = 2 \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} x\, e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}}$$

3. From working out the finite square well (FSW), $z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$. To compare to the delta function well, we take the limit as the width $a \to 0$ and the depth $V_0 \to \infty$. Because a goes to 0 faster than $\sqrt{V_0} \to \infty$, $\boxed{z_0 \to 0}$ so the delta function is a weak potential.

Let's now find the bound state energy for a δ-function well by taking this limit of a FSW. We found that the transcendental eqn. for a FSW is

$$\tan(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}, \quad \text{with } z = \frac{a}{\hbar}\sqrt{2m(E + V_0)}.$$

The RHS then equals $\sqrt{\frac{V_0}{E + V_0} - 1}$. For the LHS, we know $z_0 \to 0$, and for bound states we need $z < z_0$ (or else the RHS would be imaginary), so $z \to 0$ also. So we can use the <u>small-angle approximation</u> for tangent, <u>$\tan z \approx z$</u> (can also do a Taylor series yourself).

So we now have

$$z = \sqrt{\frac{V_0}{E + V_0} - 1}$$

(3. continued)

Back to our delta function parameters, we usually have potential $V = \alpha\delta(x)$, where α controls the strength of the well. We want the limit as the ~~both~~ FSW area approaches the area of the δ-function, which is $\int V dx = \int \alpha\delta(x)\,dx = \alpha$, so we have $2V_0 a = \alpha$,
$\Rightarrow V_0 = \frac{\alpha}{2a}$. Plugging this into our eqn above,

$$\underbrace{\frac{a}{\hbar}\sqrt{2m\left(E+\frac{\alpha}{2a}\right)}} = \underbrace{\sqrt{\frac{\frac{\alpha}{2a}}{E+\frac{\alpha}{2a}} - 1}}$$

$$\frac{1}{\hbar}\sqrt{\underset{\uparrow}{2mEa^2} + ma\alpha} = \sqrt{\frac{\alpha}{2aE+\alpha} - 1}$$

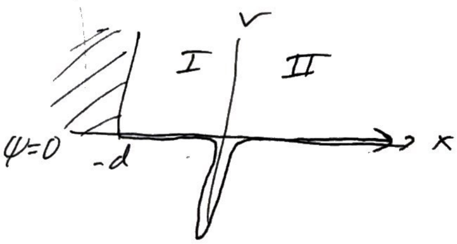
As we take the limit $a \to 0$ this term goes to zero much faster than others, so kill it; and square:

$$\frac{1}{\hbar^2}ma\alpha = \frac{\alpha}{2aE+\alpha} - 1 \quad \Rightarrow \quad \alpha = (2aE+\alpha)\left[\frac{m\alpha a}{\hbar^2} + 1\right]$$

$$\Rightarrow 2E\left(\underset{\uparrow}{\frac{ma\alpha}{\hbar^2}} + 1\right) + \frac{m\alpha^2}{\hbar^2} = 0$$

Now this term goes to 0 as $a \to 0$, so we get $\boxed{E = -\frac{m\alpha^2}{2\hbar^2}}$ This is the usual δ-function bound state solution!

4. Atom near a wall: $V = \begin{cases} x > -d: & V(x) = -V_0\delta(x) \\ x < -d: & V(x) = \infty \end{cases}$



a) Region I: $V=0$, schröd: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$

$$\Rightarrow \frac{d^2\psi}{dx^2} = \overbrace{\frac{\sqrt{-2mE}}{\hbar^2}}^{\kappa^2}\psi$$

κ^2, bc E is negative (for δ-well)

So $\boxed{\psi_I = Ae^{\kappa x} + Be^{-\kappa x}}$

Similarly for Region II, we get the same general solution, but as $x \to \infty$ we can't have $\psi_I \to \infty$ so we need the first term to be zero, thus
$\boxed{\psi_{II} = De^{-\kappa x}}$

BCs: continuity @ $x=0$: $\psi_I(0) = \psi_{II}(0) \Rightarrow A + B = D$

discontinuity @ $x=0$: By the usual procedure integrating over a region $-\epsilon$ to ϵ,

$$\underbrace{\Delta\frac{d\psi}{dx}}_{\downarrow} = -\frac{2mV_0}{\hbar^2}\underbrace{\psi(0)}_{D}$$

$$\frac{d\psi_{II}(0)}{dx} - \frac{d\psi_I(0)}{dx} = -Dk - (Ak - Bk) = k(-D-A+B)$$

$$\Rightarrow k(B-A-\underset{\uparrow \text{ here}}{D}) = -\frac{2mV_0}{\hbar^2}D \rightarrow k(B-A-(A+B)) = -2kA = -\frac{2mV_0}{\hbar^2}(A+B)$$

(4. continued)

$\Rightarrow -2k = -\frac{2mV_0}{\hbar^2}(1-e^{-2kd}) \Rightarrow \boxed{k = \frac{mV_0}{\hbar^2}(1-e^{-2kd})}$ This is the transcendental eqn. for the energy.

To estimate the energy, let's first find E^0 when d is very large – specifically, the far away wall means $kd >> 1$ (so that the term $e^{-2kd} \to 0$), and when this is the case, $k^0 = \frac{mV_0}{\hbar^2}$, so $\frac{mV_0 d}{\hbar^2} >> 1 \to \boxed{d >> \frac{\hbar^2}{mV_0}}$. We can plug this k back into the energy equation: $k = \frac{\sqrt{-2mE}}{\hbar} \to E = -\frac{\hbar^2 k^2}{2m}$, so

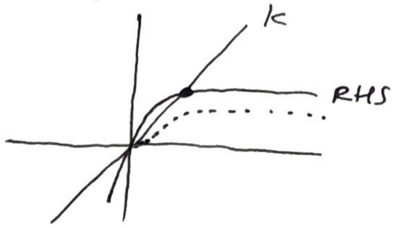
$E^0 = -\frac{\hbar^2}{2m}\left(\frac{mV_0}{\hbar^2}\right) = -\frac{mV_0^2}{2\hbar^2}$, the usual δ-function energy! (Here V_0 is analagous to α).

So then we can plug in this ~~energy~~ k to perturbatively get the next order ~~energy~~ k:

$$k' = \frac{mV_0}{\hbar^2}\left(1-e^{-2k^0 d}\right) = \frac{mV_0}{\hbar^2}\left(1-e^{-\frac{2mV_0 d}{\hbar^2}}\right)$$

$$E' = -\frac{\hbar^2(k')^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{m^2V_0^2}{\hbar^4}\right)\left(1-e^{-\frac{2mV_0 d}{\hbar^2}}\right)^2 = \boxed{-\frac{mV_0^2}{2\hbar^2}\left(1-\underbrace{2e^{-\frac{2mV_0 d}{\hbar^2}}}_{\text{This is the modification to the energy from the wall!}} + \underbrace{e^{-\frac{4mV_0 d}{\hbar^2}}}_{\text{this term is higher order so can ignore}}\right)}$$

b) Let's plot our transcendental eqn:



We see that depending on V_0 & d, the RHS may or may not cross the k line to give us a boundstate. The condition for the bound state is that the slope at $k=0$ of the RHS must be > 1:

To have ≥ 1 Boundstate:

$$\frac{\partial}{\partial k}\left[\frac{mV_0}{\hbar^2}\left(1-e^{-2kd}\right)\right] = \frac{mV_0}{\hbar^2}(2d)e^{-2kd}, \quad @\ k=0: \ \frac{2mV_0 d}{\hbar^2} > 1 \Rightarrow \boxed{V_0 d > \frac{\hbar^2}{2m}}$$

5. For a rotator in the x-y plane, we have $\hat{H} = \frac{L_z^2}{2I_z}$, & $L_z = \frac{\hbar}{i}\frac{d}{d\phi}$.

Schröd: $\frac{d^2\psi}{d\phi^2} = -\overbrace{\frac{2I_z E}{\hbar^2}}^{m^2}\psi$ w/ solution $\psi = Be^{im\phi}$, with $m = 0, \pm 1, \pm 2 \ldots$

because of the BC $\psi(\phi+2\pi) = \psi(\phi) \Rightarrow e^{im(\phi+2\pi)} = e^{im\phi} \Rightarrow e^{im2\pi} = 1$

a) The energy eigenvalues are then: $m^2 = \frac{2I_z E}{\hbar^2} \Rightarrow \boxed{E = \frac{m^2\hbar^2}{2I_z}, \ m = 0, \pm 1, \pm 2 \ldots}$

We can normalize the eigenfunctions:

$$1 = B^2\int_0^{2\pi} e^{-im\phi}e^{im\phi}\,d\phi = B^2\int_0^{2\pi} 1\,d\phi = B^2(2\pi) \Rightarrow B = \frac{1}{\sqrt{2\pi}}, \text{ so } \boxed{\psi = \frac{1}{\sqrt{2\pi}}e^{im\phi}}$$

b) Expand $\Psi(0)$: $\Psi(0) = A\sin^2\phi = A\frac{1}{2}[1-\cos(2\phi)] = \frac{A}{2}\left[1-\frac{1}{2}\left(e^{2i\phi}+e^{-2i\phi}\right)\right]$ Now in terms of eigenstates:

$\Psi(0) = \frac{A}{2}\sqrt{2\pi}\left[\psi_0 - \frac{1}{2}(\psi_2 + \psi_{-2})\right]$. For time dependence, $E_0 = 0$, $E_{\pm 2} = \pm\frac{2\hbar^2}{I_z}$, so

find A by normalization, $A = \frac{2}{\sqrt{3\pi}}$

$$\boxed{\Psi(\phi,t) = \frac{1}{\sqrt{3\pi}}\left[1-\frac{1}{2}\left(e^{2i(\phi-\frac{\hbar t}{I_z})} + e^{-2i(\phi+\frac{\hbar t}{I_z})}\right)\right]}$$ using $\Psi(t) = \sum_n c_n\psi_n e^{-\frac{iE_n t}{\hbar}}$.