Quantum Mechanics 1 – HW6

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1.The “spin-phonon” Hamiltonian:

$$H = \omega b^\dagger b + \lambda(b + b^\dagger)\sigma_x + \mu\sigma_z$$

We use a trial wavefunction: $\psi = \phi(phonons) \times \xi(spin)$ and we minimize $\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$

Let us write a general normalized spin wavefunction in the basis of eigenstates of σ_z:

$$\xi = \cos(\theta)|+\rangle + e^{i\phi}\sin(\theta)\,|-\rangle, \qquad where\colon \sigma_z|+\rangle = |+\rangle,\ \ \sigma_z|-\rangle = -|-\rangle$$

$$\langle\xi|\xi\rangle = \langle+|\cos(\theta)\cos(\theta)\,|+\rangle + \left\langle-\middle|e^{-i\varphi}\sin(\theta)\,e^{i\varphi}\sin(\theta)\,\middle|-\right\rangle = \cos^2(\theta) + \sin^2(\theta) = 1$$

$$\langle\xi|\sigma_z|\xi\rangle = \langle+|\cos(\theta)\cos(\theta)\,|+\rangle - \left\langle-\middle|e^{-i\varphi}\sin(\theta)\,e^{i\varphi}\sin(\theta)\,\middle|-\right\rangle = \cos^2(\theta) - \sin^2(\theta) = \cos(2\theta)$$

$$\langle\xi|\sigma_x|\xi\rangle = \left\langle+\middle|\cos(\theta)\,e^{i\varphi}\sin(\theta)\,\middle|+\right\rangle + \left\langle-\middle|e^{-i\varphi}\sin(\theta)\cos(\theta)\,\middle|-\right\rangle = \cos(\theta)\sin(\theta)\left(e^{i\varphi} + e^{-i\varphi}\right)$$
$$= \sin(2\theta)\cos(\phi)$$

$$\langle\psi|\psi\rangle = \langle\phi|\langle\xi|\xi\rangle|\phi\rangle = \langle\phi|\phi\rangle$$

$$\langle\psi|H|\psi\rangle = \left\langle\phi\middle|\omega b^\dagger b\langle\xi|\xi\rangle + \lambda(b + b^\dagger)\langle\xi|\sigma_x|\xi\rangle + \mu\langle\xi|\sigma_z|\xi\rangle\middle|\phi\right\rangle$$
$$= \left\langle\phi\middle|\omega b^\dagger b + \lambda(b + b^\dagger)\sin(2\theta)\cos(\phi) + \mu\cos(2\theta)\middle|\phi\right\rangle$$

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\left\langle\phi\middle|\omega b^\dagger b + \lambda(b + b^\dagger)\sin(2\theta)\cos(\phi) + \mu\cos(2\theta)\middle|\phi\right\rangle}{\langle\phi|\phi\rangle}$$
$$= \frac{1}{\langle\phi|\phi\rangle}\left\langle\phi\middle|\omega\left(b^\dagger + \frac{\lambda}{\omega}\sin(2\theta)\cos(\phi)\right)\left(b + \frac{\lambda}{\omega}\sin(2\theta)\cos(\phi)\right) - \frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2(\phi) + \mu\cos(2\theta)\middle|\phi\right\rangle$$

We define $a = b + \frac{\lambda}{\omega}\sin(2\theta)\cos(\phi)$, $a^\dagger = b^\dagger + \frac{\lambda}{\omega}\sin(2\theta)\cos(\phi)$.

We may consider $a, a^\dagger$ as ladder operators of number states since they trivially obey the bosonic commutation relations of $b, b^\dagger$

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{1}{\langle\phi|\phi\rangle}\left\langle\phi\middle|\omega a^\dagger a - \frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2(\phi) + \mu\cos(2\theta)\middle|\phi\right\rangle$$

Which represents a “shifted H-O”, the energy spectrum is thus:

$$E_n = \omega n - \frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2(\phi) + \mu\cos(2\theta), \ \ n = 0,1,2\ldots$$

We refer to $|\phi\rangle$ as an expansion in the number states of $a, a^\dagger$

It is obvious that the lowest energy state will be given by $|\phi_0\rangle = |0\rangle$:

$$E_0 = -\frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2(\phi) + \mu\cos(2\theta)$$

We find its absolute minimum by varying θ, ϕ:

$$0 = \frac{\partial E_0}{\partial\theta} = -4\frac{\lambda^2}{\omega}\sin(2\theta)\cos(2\theta)\cos^2(\phi) - 2\mu\sin(2\theta) = -2\sin(2\theta)\left(2\frac{\lambda^2}{\omega}\cos(2\theta)\cos^2(\phi) + \mu\right)$$

$$0 = \frac{\partial E_0}{\partial\varphi} = 2\frac{\lambda^2}{\omega}\sin^2(2\theta)\cos(\phi)\sin(\phi) = \frac{\lambda^2}{\omega}\sin^2(2\theta)\sin(2\phi)$$

case A: $\sin(2\theta) = 0 \;\rightarrow\; 2\theta = \pi k, k \in \mathbb{N} \;\rightarrow\; \theta = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$

case B: $2\frac{\lambda^2}{\omega}\cos(2\theta)\cos^2(\phi) + \mu = 0 \;\rightarrow\; \cos(2\theta)\cos^2(\phi) = -\frac{\mu\omega}{2\lambda^2}$

$$\sin(2\phi) = 0 \;\rightarrow\; 2\phi = \pi k, k \in \mathbb{N} \;\rightarrow\; \phi = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$$

If we plug $\phi = \frac{\pi}{2}, \frac{3\pi}{2}$ then $\cos^2(\phi) = 0$ so the 1st condition is: $0 = -\frac{\mu\omega}{\lambda^2}$ which we cannot impose.
If we plug $\phi = 0, \pi$ then $\cos^2(\phi) = 1$ so the 1st condition is: $\cos(2\theta) = -\frac{\mu\omega}{2\lambda^2}$ only in the regime where: $\left|\frac{\mu\omega}{2\lambda^2}\right| \leq 1$, otherwise it is not an extremum.

We now find E_0 in all suspected extremum cases

case A: $\theta = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$ and $0 \leq \phi < 2\pi$

$$E_0 = -\frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2(\phi) + \mu\cos(2\theta) = \begin{cases} +\mu & \theta = 0, \pi \quad | \, 0 \leq \phi < 2\pi \\ -\mu & \theta = \frac{\pi}{2}, \frac{3\pi}{2} \;\; | \, 0 \leq \phi < 2\pi \end{cases}$$

case B: $\phi = 0, \pi$ and $\cos(2\theta) = -\frac{\mu\omega}{2\lambda^2}$

$$\begin{aligned} E_0 &= -\frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2(\phi) + \mu\cos(2\theta) = -\frac{\lambda^2}{\omega}\left(1 - \cos^2(2\theta)\right) + \mu\cos(2\theta) \\ &= -\frac{\lambda^2}{\omega}\left(1 - \frac{\mu^2\omega^2}{4\lambda^4}\right) - \mu\frac{\mu\omega}{2\lambda^2} = -\frac{\lambda^2}{\omega} - \frac{\mu^2\omega}{4\lambda^2} \end{aligned}$$

To conclude:

$$E_0 = \begin{cases} +\mu & \theta = 0, \pi \quad 0 \leq \phi < 2\pi \\ -\mu & \theta = \frac{\pi}{2}, \frac{3\pi}{2} \quad 0 \leq \phi < 2\pi \\ -\frac{\lambda^2}{\omega} - \frac{\mu^2\omega}{4\lambda^2} & \cos(2\theta) = -\frac{\mu\omega}{2\lambda^2} \quad \phi = 0, \pi \quad \left|\frac{\mu\omega}{2\lambda^2}\right| \leq 1 \; only \end{cases}$$

We divide the problem into the regimes of the parameters:

$\boxed{\text{For } \left|\frac{\mu\omega}{2\lambda^2}\right| > 1}$ case B is no longer a suspected extremum
minimal energy is $-|\mu|$
and $|\xi_{min}\rangle$ is given by setting $\theta = \frac{\pi}{2}, \frac{3\pi}{2}$ if $\mu > 0$ and setting $\theta = 0, \pi$ if $\mu < 0$

$$|\psi_0\rangle = |\xi_{min}\rangle|\phi_0\rangle = \begin{cases} |-\rangle|0\rangle \;, \mu > 0 \\ |+\rangle|0\rangle \;, \mu < 0 \end{cases} \; up \; to \; any \; global \; phase$$

The degeneracy is 1.

$\boxed{\text{For } \left|\frac{\mu\omega}{2\lambda^2}\right| = 1}$ which translates to $\frac{\lambda^2}{\omega} = \frac{1}{2}|\mu|$ so we find that:

$$-\frac{\lambda^2}{\omega} - \frac{\mu^2\omega}{4\lambda^2} = -\frac{1}{2}|\mu| - \frac{\mu^2 2}{4|\mu|} = -\frac{1}{2}|\mu| - \frac{1}{2}|\mu| = -|\mu|$$

So the energies $-\frac{\lambda^2}{\omega} - \frac{\mu^2\omega}{4\lambda^2}$ and $-|\mu|$ coincide to 1 minima. The state corresponding to energy $-|\mu|$ is given by $|\psi_0\rangle$, let us find the states corresponding to energy $-\frac{\lambda^2}{\omega} - \frac{\mu^2\omega}{4\lambda^2}$

we get $|\xi_{min}\rangle$ by setting $\phi = 0, \pi$

$$\& \ \theta = \frac{1}{2}\text{acos}\left(-\frac{\mu\omega}{2\lambda^2}\right) = \frac{1}{2}\begin{cases}\text{acos}(-1) & ,\mu > 0\\ \text{acos}(1) & ,\mu < 0\end{cases} = \frac{1}{2}\begin{cases}\pi, 3\pi & ,\mu > 0\\ 0, 2\pi & ,\mu < 0\end{cases}$$

The possible values of θ give exactly the separation we got for $|\psi_0\rangle$ and it will trivially lead to the same wavefunction according to the sign of μ. So there is no degeneracy here and the wavefunction is

$$|\psi_0\rangle = |\xi_{min}\rangle|\phi_0\rangle = \begin{cases}|-\rangle|0\rangle & ,\mu > 0\\ |+\rangle|0\rangle & ,\mu < 0\end{cases} \ \textit{up to any global phase}$$

$\boxed{\text{For } \left|\frac{\mu\omega}{2\lambda^2}\right| < 1}$ which translates to $\frac{\lambda^2}{\omega} > \frac{1}{2}|\mu|$we find that: $-\frac{\lambda^2}{\omega} - \frac{\mu^2\omega}{4\lambda^2} < -|\mu|$ so the minimal energy is $-\frac{\lambda^2}{\omega} - \frac{\mu^2\omega}{4\lambda^2}$ corresponding to the following states:

selecting $\phi = 0, \theta = \ \theta' = \frac{1}{2}\text{acos}\left(-\frac{\mu\omega}{2\lambda^2}\right)$:

$$|\psi_2\rangle = |\xi_{min}^{+}\rangle|\phi_0\rangle = (\cos(\theta')|+\rangle + \sin(\theta')\,|-\rangle)|0\rangle \ \textit{up to global phase}$$

selecting $\phi = \pi, \theta = \ \theta'$:

$$|\psi_3\rangle = |\xi_{min}^{-}\rangle|\phi_0\rangle = (\cos(\theta')|+\rangle - \sin(\theta')\,|-\rangle)|0\rangle \ \textit{up to global phase}$$

Here we got a 2-fold degeneracy in the ground state.

2. The Hartree Fock equation for N Fermions.
Let ψ_t be a trial wavefunction of the N fermions. $\psi_t = \psi_t(\phi_1, \phi_2 \dots, \phi_N)$
We wish to minimize $\langle\psi_t|H|\psi_t\rangle$ under the condition $\int|\phi_\alpha(\vec{r})|^2 d^3r = 1$.
Taking the variational derivative of ϕ_α^*, as we did in class, one gets for translational invariant system:

$$h_f\phi_\gamma(\vec{r}) + \int u(\vec{r}-\vec{r}^{\,'}) \sum_{\beta\in occ} \left|\phi_\beta(\vec{r}^{\,'})\right|^2 d^3r'\,\phi_\gamma(r)$$

$$- \int u(\vec{r}-\vec{r}^{\,'}) \left(\sum_{\beta\in occ} \delta_{s_\gamma s_\beta} \phi_\beta^*(\vec{r}^{\,'})\phi_\beta(\vec{r}) \right) \phi_\gamma(\vec{r}^{\,'}) d^3r' = \varepsilon_\gamma \phi_\gamma(\vec{r})$$

We simply plug the plane wave solution: $\phi_\gamma(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\mathrm{k}\cdot\mathrm{r}}$

$$\frac{\hbar^2k^2}{2m}\frac{1}{\sqrt{V}}e^{i\mathrm{k}\cdot\mathrm{r}} + \int u(\vec{r}-\vec{r}^{\,'})\frac{N}{V}d^3r'\frac{1}{\sqrt{V}}e^{i\mathrm{k}\cdot\mathrm{r}} - \sum_{,k',s'\in occ} \delta_{s',s}\int u(\vec{r}-\vec{r}^{\,'})\frac{1}{V}e^{i(\mathrm{k}-\mathrm{k}')\cdot\mathrm{r}'}d^3r'\frac{1}{\sqrt{V}}e^{i\mathrm{k}'\cdot\mathrm{r}}$$

$$= \frac{\hbar^2k^2}{2m}\frac{1}{\sqrt{V}}e^{i\mathrm{k}\cdot\mathrm{r}} + \frac{N}{V}\int u(\vec{r}-\vec{r}^{\,'})d^3r'\frac{1}{\sqrt{V}}e^{i\mathrm{k}\cdot\mathrm{r}} - \frac{1}{V}\sum_{k',s'\in occ} \delta_{s',s}\int u(\vec{r}-\vec{r}^{\,'})e^{i(\mathrm{k}-\mathrm{k}')\cdot(\mathrm{r}'-\mathrm{r})}d^3r'\frac{1}{\sqrt{V}}e^{i\mathrm{k}\cdot\mathrm{r}}$$

$$= \varepsilon_k \frac{1}{\sqrt{V}}e^{i\mathrm{k}\cdot\mathrm{r}}$$

Notice that: $\int u(\vec{r}-\vec{r}^{\,'})d^3r' = \bar{u}(0)$, $\int u(\vec{r}-\vec{r}^{\,'})e^{i(\mathrm{k}-\mathrm{k}')\cdot(\mathrm{r}'-\mathrm{r})}d^3r' = \bar{u}(\mathrm{k}-\mathrm{k}')$, where $\bar{u}$ is the Fourier Transform of u.
Also: $\Sigma_{k',s'\in occ} = N$ wheras $\Sigma_{k',s'\in occ}\delta_{s',s} \neq N$ because we only sum over particles with same spin.
So the plane wave is indeed a solution, and we end up with the single particle spectrum:

$$\varepsilon_k = \frac{\hbar^2k^2}{2m} + \frac{N}{V}\bar{u}(0) - \frac{1}{V}\sum_{k',s'\in occ} \delta_{s',s}\bar{u}(\mathrm{k}-\mathrm{k}')$$

3. Asymmetric potential well.

At $t = 0$ we choose the left well to be the lowest of the two and, as the question implies, we consider the wavefunction to be at the ground-state of the left well. This consideration is valid ofcourse, only when one considers the barrier and width (distance between left and right bottoms) large enough so that there is no substantial overlap and therefore the ground state of the entire system is that of the left (lowest) well.

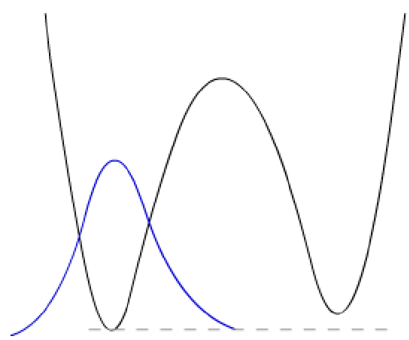
As time evolves the left well rises as the right well descends, in the extreme adiabatic approximation we consider this process very slow so that at any given time the system chooses its complete ground state. I will interpret "very slow" quantitatively later on.

Let t^* be the time for which the ground state energies of the two wells coincide.

$$\varepsilon_0^L(t^*) = \varepsilon_0^R(t^*)$$

For $t < t^* - dt$, namely- as long as the left well is lower than the right well, the system holds on to the ground state of the left well as its wf changes adiabitaclly because the barrier grows smaller

$$\psi(t) = \varphi_0^L(t), \qquad t < t^* - dt$$



During this stage "very slow" would mean that the energy gap between the ground state of the left well and its first excited state or the gap between the left ground state and the right ground state are big enough so that the characteristic time in which the wavefunction $\varphi_0^L(t)$ changes is much larger than $\hbar/\Delta E$, to put it more quantitatively, let us approximate the left well to a Harmonic Oscillator at its bottom curve and get $\omega^L(t)$ from the second derivative of the potential in the minimum point.

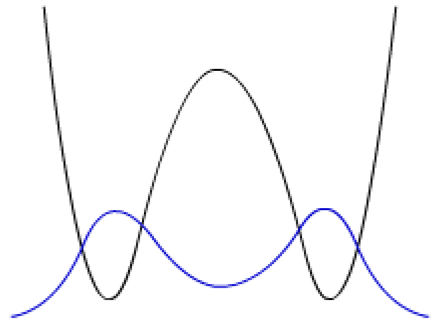
The characteristic time is $\tau^L \sim \frac{1}{\omega^L(t)}$

We define $\Delta E_{01}^L = \varepsilon_1^L(t) - \varepsilon_0^L(t), \quad \Delta E_0^{RL} = \varepsilon_0^R(t) - \varepsilon_0^L(t)$ and require:

$$\tau^L \gg \frac{\hbar}{\Delta E_{01}^L}, \qquad \tau^L \gg \frac{\hbar}{\Delta E_0^{RL}}$$

This limit will ensure that $\psi(t) = \varphi_0^L(t)$ for $t < t^* - dt$. (Born Openheimer approx)

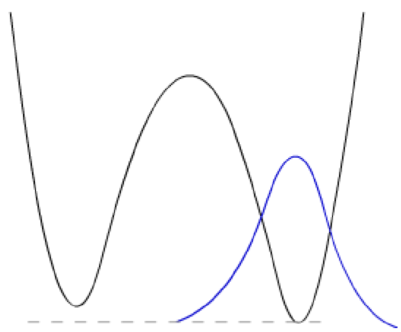
At $t = t^*$ there is a degeneracy at the ground state: $\frac{1}{\sqrt{2}}\left(\varphi_o^L(t^*) \pm \varphi_0^R(t^*)\right)$
The degeneracy is broken in perturbation theory so that the system chooses the + sign wf as the ground state.



This transition between $\psi(t^* - dt) = \varphi_0^L(t - dt)$ to $\psi(t^*) = \frac{1}{\sqrt{2}}\left(\varphi_o^L(t^*) + \varphi_0^R(t^*)\right)$ can happen only if we consider a "very slow" process in which dt is large enough so that the system may significantly change its position space dependence.
Between t^* and $t^* + dt$ the same idea works in reverse only to arrive at the ground state energy of the right-hand well $\psi(t^* + dt) = \varphi_0^R(t^* + dt)$ which will be the new ground state of the system.

For $t > t^* + dt$ the system holds on to ground state of the right well as it changes adiabatically, like it did before in the left well ground state.

$$\psi(t) = \varphi_0^R(t), \qquad t > t^* + dt$$



And similarly we want the B-O approximation to hold so that: $\tau^R \gg \frac{\hbar}{\Delta E_{01}^R}$, $\tau^R \gg \frac{\hbar}{\Delta E_0^{LR}}$

4. To use the B-O approximation we'll look for a "fast" coordinate and "slow" coordinate.
Notice that treating y as a slow coordinate, taking it as a fixed parameter as we solve the problem for the $\hat{x}$ axis alone we get eigen energies of infinite well proportional to $\frac{1}{a^2}$ which are much higher then what we would have gotten had we treated this problem the other way around (for y we get small energies proportional to $\frac{1}{b^2}$)
We know that the eigen-energies correspond to the frequency of the wavefunction and we therefore conclude that under $a \ll b$ it will be safe to consider x the fast coordinate, and y as slow.

Let $\phi(x; y)$ be the fast coordinate (i.e x) wavefunction given that the width of the infinite well is determined by the slow varying coordinate y.
The potential is zero when: $\frac{x^2}{a^2} + \frac{y^2}{b^2} < 1 \rightarrow x^2 < a^2\left(1 - \frac{y^2}{b^2}\right) \rightarrow -a\sqrt{1 - \frac{y^2}{b^2}} < x < a\sqrt{1 - \frac{y^2}{b^2}}$ and infinite otherwise. We define $a(y) = a\sqrt{1 - \frac{y^2}{b^2}}$
The eigenfunctions and energies of the x infinite well are thus.

$$\phi_n(x; y) = \begin{cases} \sqrt{\dfrac{2}{2a(y)}} \sin\left(\dfrac{\pi n}{2a(y)}\big(x + a(y)\big)\right) & x^2 < a^2(y) \\ 0 & x^2 > a^2(y) \end{cases} \qquad \varepsilon_n(y) = \frac{\hbar^2\pi^2 n^2}{8ma^2(y)}$$

We write the total wavefunction:

$$\psi = \sum_n \xi_n(y)\phi_n(x; y)$$

The effective Hamiltonian that now works on y in the B-O approximation is:

$$H_n^{BO} = \frac{1}{2m}\big(p_y + iA_n(y)\big)^2 + V_n^{eff}(y)$$

Where: $A_n = \left\langle \phi_n \middle| \frac{\partial}{\partial y} \middle| \phi_n \right\rangle$ is pure imaginary and ϕ_n are real so: $A_n(y) = 0$ (N0 vector potential term)

And: $V_n^{eff} \approx \begin{cases} \varepsilon_n(y) & y^2 < b^2 \\ \infty & y^2 > b^2 \end{cases}$

We solve $H_n^{BO}\xi_n(y) = E\xi_n(y)$ in the well:

$$\rightarrow \left(\frac{p_y^2}{2m} + \frac{\hbar^2\pi^2 n^2}{8ma^2(y)}\right)\xi_n(y) = E\xi_n(y)$$

Approximating $\frac{1}{a^2(y)} = \frac{1}{a^2\left(1 - \frac{y^2}{b^2}\right)}$ under $y \ll b$ to get a fairly solvable problem:

$$\frac{1}{a^2\left(1 - \frac{y^2}{b^2}\right)} \approx \frac{1}{a^2}\left(1 + \frac{y^2}{b^2}\right)$$

$$\rightarrow \left(\frac{p_y^2}{2m} + \underbrace{\frac{\hbar^2\pi^2 n^2}{8ma^2}}_{const} + \frac{\hbar^2\pi^2 n^2}{8ma^2}\frac{y^2}{b^2}\right)\xi_n(y) = E\xi_n(y)$$

Noticing that $\frac{\hbar^2\pi^2 n^2}{8ma^2} = \varepsilon_n(0)$ and denoting: $\frac{1}{2}m\omega_n^2 = \frac{\hbar^2\pi^2 n^2}{8ma^2b^2}$ (i.e $\omega_n = \frac{\hbar\pi n}{2mab}$)

$$\rightarrow \left(\frac{p_y^2}{2m} + \frac{1}{2}m\omega_n^2 y^2 + \varepsilon_n(0)\right)\xi_n(y) = E\xi_n(y)$$

For any n this is a H-O in coordinate y with shifted energy by a constant $\varepsilon_n(0)$, giving the lower part of the spectrum (small l's and n's):

$$E_{n,l} = \hbar\omega_n\left(l + \frac{1}{2}\right) + \varepsilon_n(0) = \frac{\hbar^2\pi n}{2mab}\left(l + \frac{1}{2}\right) + \frac{\hbar^2\pi^2 n^2}{8ma^2}, \qquad n, l \in \mathbb{N}$$

Corresponding eigen wavefunctions:

$$\psi_{n,l} = \xi_{n,l}^{HO}(y)\phi_n^{Well}(x;y) = \frac{1}{\sqrt{2^l l!}} \cdot \left(\frac{m\omega_n}{\pi\hbar}\right)^{\frac{1}{4}} \cdot \exp\left(-\frac{m\omega_n y^2}{2\hbar}\right) \cdot H_l\left(\sqrt{\frac{m\omega_n}{\hbar}}y\right) \cdot \phi_n(x;y)$$

Where H_l are the Hermite polynomials and recalling that:

$$\omega_n = \frac{\hbar\pi n}{2mab}, \qquad \phi_n(x;y) = \begin{cases} \sqrt{\frac{2}{2a(y)}}\sin\left(\frac{\pi n}{2a(y)}\left(x + a(y)\right)\right) & x^2 < a^2(y) \\ 0 & x^2 > a^2(y) \end{cases}, \qquad a(y) = a\sqrt{1 - \frac{y^2}{b^2}}$$