Physics 492: Quantum Mechanics II

Problem Set #3: Solutions

Problem 1: Center of mass and relative coordinates

We consider two particles moving along the x-axis.

We know that operators associated with different degrees commute.

$$[\hat{x}_i, \hat{x}_j] = 0 \qquad [\hat{p}_i, \hat{p}_j] = 0 \qquad [\hat{x}_i, \hat{p}_j] = i\hbar\, \delta_{ij}$$

We now consider the center-of-mass are relative coordinates

$$\hat{X}_{CoM} = \frac{m_1 \hat{x}_1 + m_2 \hat{x}_2}{m_1 + m_2}, \qquad \hat{P}_{CoM} = \hat{p}_1 + \hat{p}_2$$

$$\hat{x}_{rel} = \hat{x}_1 - \hat{x}_2, \qquad \hat{p}_{rel} = \frac{m_2 \hat{p}_1 - m_1 \hat{p}_2}{m_1 + m_2}$$

(a) $[\hat{X}_{CoM}, \hat{P}_{CoM}] = \frac{m_1}{m_1+m_2}[\hat{x}_1, \hat{p}_1] + \frac{m_2}{m_1+m_2}[\hat{x}_2, \hat{p}_2] = i\hbar\left(\frac{m_1+m_2}{m_1+m_2}\right) = i\hbar$

$[\hat{x}_{rel}, \hat{p}_{rel}] = \frac{m_2}{m_1+m_2}[\hat{x}_1, \hat{p}_1] + \frac{-m_1}{m_1+m_2}[\hat{x}_2, \hat{p}_2] = i\hbar\left(\frac{m_1+m_2}{m_1+m_2}\right) = i\hbar$

$[\hat{X}_{CoM}, \hat{p}_{rel}] = \frac{m_1 m_2}{(m_1+m_2)^2}[\hat{x}_1, \hat{p}_1] - \frac{m_1 m_2}{(m_1+m_2)^2}[\hat{x}_2, \hat{p}_2] = 0$

$[\hat{x}_{rel}, \hat{P}_{CoM}] = [\hat{x}_1, \hat{p}_1] - [\hat{x}_2, \hat{p}_2] = 0$

$\Rightarrow$ Center of mass and relative-coordinates are different degrees of freedom.

(b) If both particles are free particles, then $\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m}$ (sum of kinetic energies of the two particles).

Now $\hat{p}_1 = \frac{m_1}{M}\hat{P}_{CoM} + \hat{p}_{rel}$, $\hat{p}_2 = \frac{m_2}{M}\hat{P}_{CoM} - \hat{p}_{rel}$, where $M = m_1 + m_2$

$$\Rightarrow \hat{p}_1^2 = \frac{m_1^2}{M^2}\hat{p}_{CoM}^2 + \frac{2m_1}{M}\hat{p}_{CoM}\hat{p}_{rel} + \hat{p}_{rel}^2 , \quad \hat{p}_2^2 = \frac{m_2^2}{M^2}\hat{p}_{CoM}^2 - \frac{2m_2}{M}\hat{p}_{CoM}\hat{p}_{rel} + \hat{p}_{rel}^2$$

$$\Rightarrow \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} = \frac{1}{2}\left(\frac{m_1+m_2}{M^2}\right)\hat{p}_{CoM}^2 + \frac{1}{2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\hat{p}_{rel}^2 = \frac{\hat{p}_{CoM}^2}{2M} + \frac{\hat{p}_{rel}^2}{2\mu}$$

Where $\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \Rightarrow \mu = \frac{m_1 m_2}{m_1+m_2}$ = reduced mass

(c) Kinetic energy separates also in Center-of-mass and relative coordinates. We can understand this from the point of view of translation symmetry. There are no center-of-mass or relative forces.

Now consider a two-particle state whose wave function in the position representation is $\Psi(x_1, x_2) = \delta(x_2 - x_1 - X_0)$

(d) In momentum space: $\tilde{\Phi}(p_1,p_2) = \int\frac{dx_1}{\sqrt{2\pi\hbar}}\int\frac{dx_2}{\sqrt{2\pi\hbar}}\,\Psi(x_1,x_2)\, e^{-\frac{ip_1x_1}{\hbar}}\, e^{-\frac{ip_2x_2}{\hbar}}$

$$\Rightarrow \Phi(p_1,p_2) = \int\frac{dx_1}{2\pi\hbar}\, e^{-\frac{ip_1x_1}{\hbar}}\, e^{-\frac{ip_2(x_1+X_0)}{\hbar}} = e^{-\frac{ip_2X_0}{\hbar}}\int\frac{dx_1}{2\pi\hbar}\, e^{-\frac{i(p_1+p_2)x_1}{\hbar}}$$

$$= e^{-\frac{ip_2X_0}{\hbar}}\,\delta(p_1+p_2)$$

(e) We thus see $\hat{x}_{rel}\Psi(x_1,X_2) = X_0\,\Psi(x_1,x_2)$: Relative position $= X_0$

$\hat{P}_{CoM}\,\tilde{\Phi}(p_1,p_2) = 0$ CoM momentum $=0$

This state is consistent with the uncertainty principle since $\hat{x}_{rel}$ and $\hat{P}_{CoM}$ commute.

Problem # 2.: 1D, 2D, 3D

(a) A particle is confined in two directions and free in the third.

In the x-y plane: $V(x,y) = \begin{cases} 0, & 0<x<a_x,\ 0<y<a_y \\ \infty, & \text{otherwise} \end{cases}$

Free along z.

The Hamiltonian $\hat{H} = \frac{|\hat{\vec{p}}|^2}{2m} + V(x,y)$

$$= \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + V(x,y) + \frac{\hat{p}_z^2}{2m}$$

Since the infinite square well in 2D is separable, the Hamiltonian is separable in x, y, z

$$\hat{H} = \underbrace{\hat{H}^{(x)} + \hat{H}^{(y)}}_{\text{2D well}} + \underbrace{\hat{H}^{(z)}}_{\text{Free along } z} : \frac{\hat{p}_z^2}{2m}$$

$\Rightarrow$ Energy eigenvalues: $E = E^{(x)} + E^{(y)} + E^{(z)}$

Along each direction $E^{(j)} = \frac{(\hbar k_j)^2}{2m}$

In the x-y directions, the energy is quantized while along z, k_z can take any value

$$\Rightarrow \boxed{E_{n_x,n_y}(k_z) = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) \qquad k_x = n_x \frac{\pi}{a_x} \quad k_y = n_y \frac{\pi}{a_y}}$$

Eigenfunctions of $\hat{H}$ = product of 1D eigenfunctions

$$\psi_{n_x, n_y, k_z}(\vec{x}) = \left[\sqrt{\frac{2}{a_x}}\, \sin\left(n_x \frac{\pi}{a_x} x\right)\right]\left[\sqrt{\frac{2}{a_y}}\, \sin\left(n_y \frac{\pi}{a_y} y\right)\right]\left(\frac{e^{ik_z z}}{\sqrt{2\pi}}\right)$$

Degeneracy? Though the state depends on n_x, n_y and k_z independently, the energy only depends on the sum $k_x^2 + k_y^2 + k_z^2$

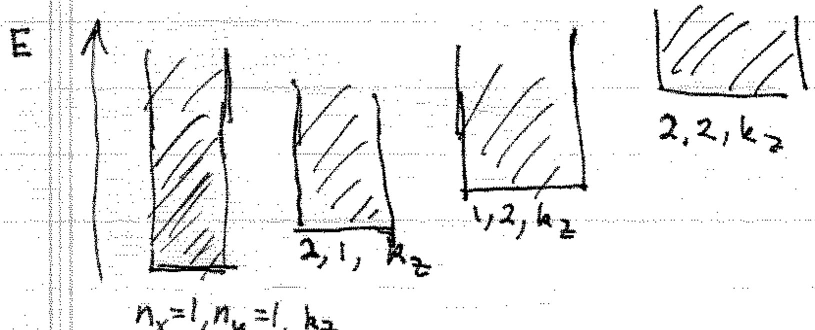
$$= \pi^2 \frac{\hbar^2}{2ma_x^2}\left(n_x^2 + n_y^2 \frac{a_x^2}{a_y^2}\right) + k_z^2$$

The degeneracy will always be at least $\underline{2}$: since the states $e^{+ik_z z}$ and $e^{-ik_z z}$ are degenerate this gives one factor of 2 (this is an essential degeneracy due to parity). In addition, there will be another factor of 2 degeneracy for two states such that

$$E_{n_x, n_y, k_z} = E_{m_x, m_y, q_z}$$

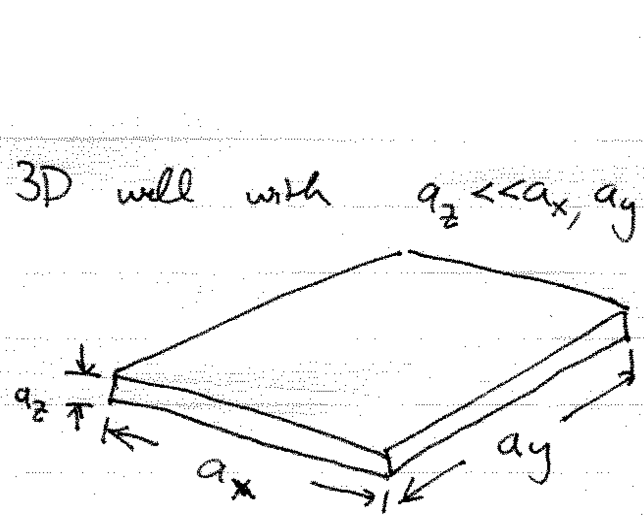
There is a continuum of such states (highly degenerate)

Sketch energy level diagram (depends on a_x and a_y)



Finally if $\frac{a_x}{a_y}$ = rational # there will be further degeneracies.

(b) 3D well with $a_z \ll a_x, a_y$: Slab geometry



Let us choose

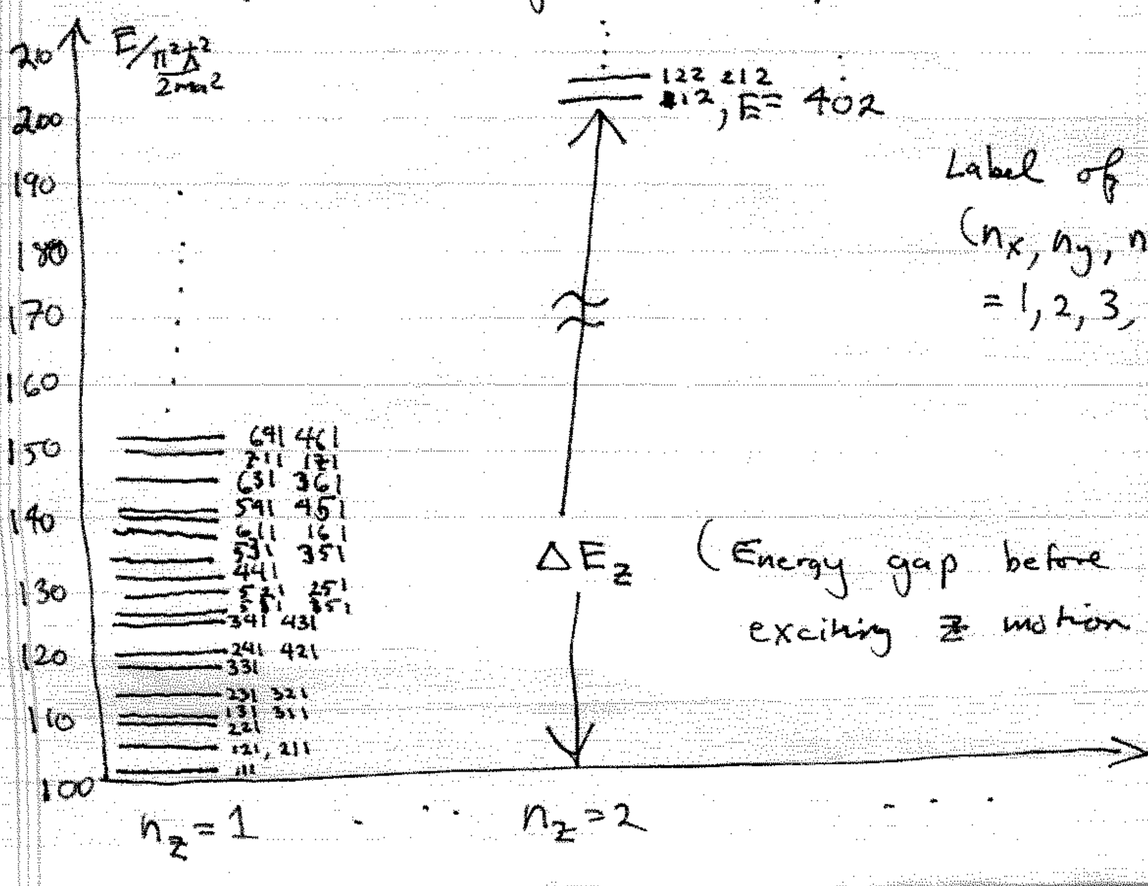
$a_x = a_y \equiv a_z$

$a_z = \frac{a}{10}$

$$\Rightarrow E_{n_x, n_y, n_z} = \frac{\pi^2 \hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + 100 n_z^2\right)$$

All states with $n_x \neq n_y$ are doubly degenerate since we can switch $n_x \Leftrightarrow n_y$ (essentiall degneracy). In addition, when n_x or $n_y = 10 n_z$ there is another degeneracy.

Sketch of level diagram (rough)



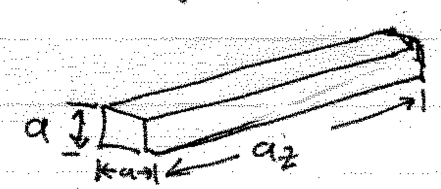
Label of levels

$(n_x, n_y, n_z) = 1, 2, 3, \ldots$

Comment: Due to the uncertainty principle, tight confinement along z implies a large energy gap for excitation of motion along z.

(c) Now we consider a "wire" geometry with

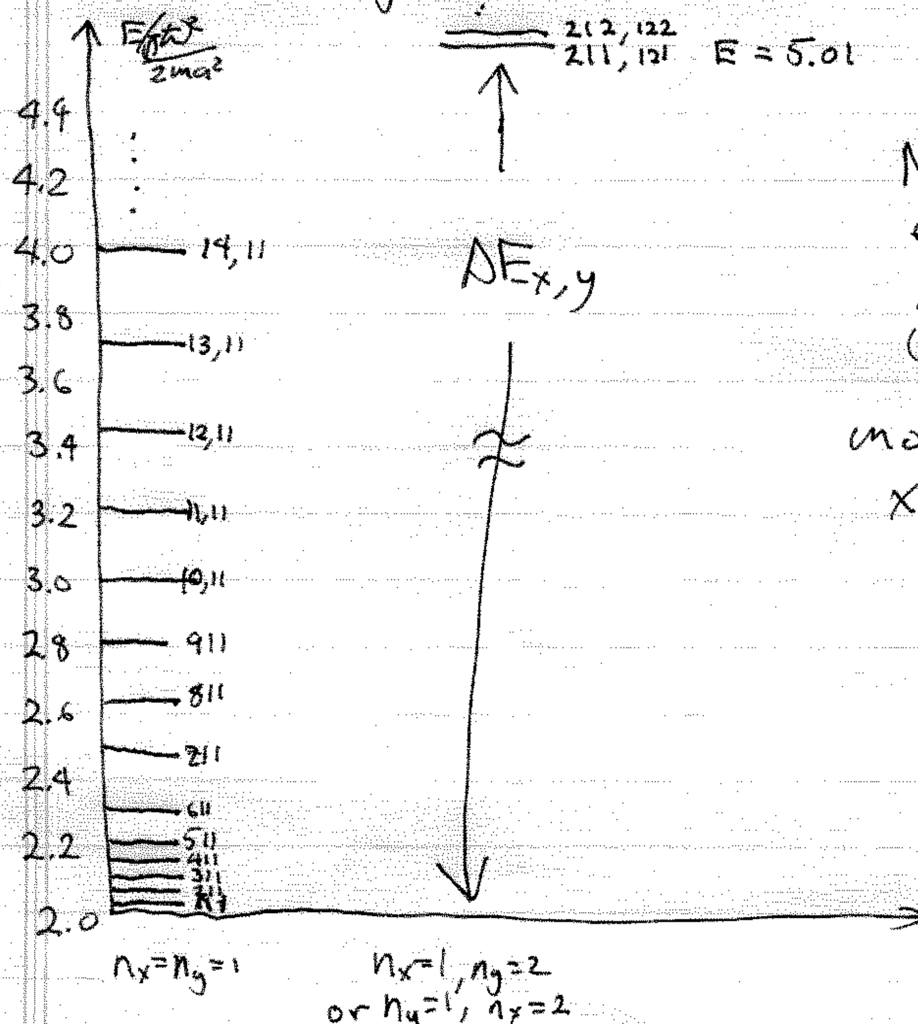
$$a_x = a_y \equiv a \qquad a_z = \frac{a}{10} << a_x, a_y$$



$$E = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + \frac{n_z^2}{100}\right)$$

Again, states with $n_x \neq n_y$ are doubly degenerate. There are additional degeneracies when $n_z = 10n_x$ or $10n_y$

Sketch energy level diagram



Now the energy gap exists for exciting motion along x or y

(d) We would like to "engineer" a system which behaves as a reduced dimensional system. To do this we want to allow excitations of motion in some directions and lock out motion in the others. We can achieve this by noticing that in confined geometries there is a large energy gap to exciting motion in the confined direction(s). ~~Remem~~ Remember that in thermal equilibrium, the probability of excitation with energy $E \propto e^{-E/k_B T}$

Where k_B = Boltzmann's constant, T = temperature.

Thus, we want to cool the system to temperatures $T \ll \Delta E_{gap}/k_B$. There are many energy levels associated with motion along the weakly confined directions. Thus, we can see dynamics in the unconfined directions, and lock out any motion along the confined directions

This kind of engineering is now applied to electrons in semiconductors

2D $\Rightarrow$ Quantum Well

1D $\Rightarrow$ Quantum Wire