# Quantum Mechanics - I: HW 5 Solutions

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## 1 Problem 1

To find the coordinate representation of the evolution operator for a free particle one must integrate over all paths. The tricky part here is coming up with a way of counting them. This can only be done by discretized the path into $N$-steps, that take time $\epsilon$. Then we integrate over the possible locations the particle can be after each interval. Before we can take the path integral we must find the action for each infinitestmal step.

$$S = \frac{1}{2}\int_t^{t+\Delta t} mv^2 = \frac{1}{2}\int_t^{t+\Delta t} m\left(\frac{\delta x}{\delta t}\right)^2 dt = \frac{m\left(\Delta x\right)^2}{2\Delta t} \tag{1}$$

Breaking the path integral into tiny bits and plugging the action above we get

$$U_0\left(x_N, x_0; t, 0\right) = \sqrt{\frac{m}{2\pi\imath\hbar\epsilon}}\int_{-\infty}^{\infty} dx_{N-1}A\cdots\int_{-\infty}^{\infty} dx_1 A e^{\frac{\imath m\left(x_N - x_{N-1}\right)^2}{2\hbar\epsilon}} e^{\frac{\imath m\left(x_{N-1} - x_{N-2}\right)^2}{2\hbar\epsilon}}\cdots e^{\frac{\imath m\left(x_1 - x_0\right)^2}{2\hbar\epsilon}} \tag{2}$$

Since these integrals can be separated into a product of integrals one can write

$$U_0\left(x, x''; t, t''\right) = \int_{-\infty}^{\infty} dx' U_0\left(x, x'; t, t'\right) U_0\left(x', x''; t', t\right) \tag{3}$$

where,

$$U_0\left(x, x'; t, t'\right) = \sqrt{\frac{m}{2\pi\imath\hbar\underbrace{\left(t' - t''\right)}_{\epsilon'}}} e^{\frac{\imath m\left(x - x'\right)^2}{2\hbar\epsilon'}} \tag{4}$$

We can show that these evolution operators form a close group, by calculating the product of two of them and showing that it gives us a evolution operator back.

$$U_0\left(x, x''; t, t''\right) = \int_{-\infty}^{\infty} dx' \sqrt{\frac{m}{2\pi\imath\hbar\left(t - t'\right)}}\sqrt{\frac{m}{2\pi\imath\hbar\left(t' - t''\right)}} e^{\frac{\imath m}{2\hbar}\left(\frac{x^2}{\epsilon'} - \frac{2xx'}{\epsilon'} + \frac{x'^2}{\epsilon'} + \frac{x'^2}{\epsilon''} - \frac{2x'x''}{\epsilon''} + \frac{x''^2}{\epsilon''}\right)} \tag{5}$$

$$= A'A'' e^{\frac{\imath m}{2\hbar}\left(\frac{x^2}{\epsilon'} + \frac{x''^2}{\epsilon''}\right)} \int_{\infty}^{\infty} dx' e^{\frac{\imath m}{2\hbar}\left(\frac{\epsilon' + \epsilon''}{\epsilon'\epsilon''}\right)x'^2} e^{-\frac{\imath m}{\hbar}\left(\frac{x}{\epsilon'} + \frac{x''}{\epsilon''}\right)x'} \tag{6}$$

using

$$\int_{-\infty}^{\infty} dx e^{-\frac{a}{2}x^2+hx} = \sqrt{\frac{2\pi}{a}} e^{\frac{h^2}{2a}} \tag{7}$$

$$U_0\left(x, x''; t, t''\right) = A'A'' e^{\frac{\imath m}{2\hbar}\left(\frac{x^2}{\epsilon'}+\frac{x''^2}{\epsilon''}\right)} \sqrt{\frac{2\pi\hbar\epsilon'\epsilon''}{\imath m\left(\epsilon'+\epsilon''\right)}} e^{\frac{m^2}{2\hbar^2}\left(\frac{x}{\epsilon'}+\frac{x''}{\epsilon''}\right)^2 \frac{\hbar\epsilon'\epsilon''}{\imath m\left(\epsilon'+\epsilon''\right)}} \tag{8}$$

$$= \sqrt{\frac{m}{2\pi\imath\hbar\epsilon'}} \sqrt{\frac{m}{2\pi\imath\hbar\epsilon''}} \sqrt{\frac{2\pi\hbar\epsilon'\epsilon''}{-\imath m\left(\epsilon'+\epsilon''\right)}} e^{\frac{\imath m}{2\hbar}\left(\frac{x^2}{\epsilon'}+\frac{x''^2}{\epsilon''}\right)} e^{-\frac{\imath m\epsilon'\epsilon''}{2\hbar\left(\epsilon'+\epsilon''\right)}\left(\frac{x^2}{\epsilon'^2}+\frac{x''^2}{\epsilon''^2}+\frac{2xx''}{\epsilon'\epsilon''}\right)} \tag{9}$$

$$= \sqrt{\frac{m}{2\pi\imath\hbar\left(\epsilon'+\epsilon''\right)}} e^{\frac{\imath m\left(x-x''\right)^2}{2\hbar\left(\epsilon'+\epsilon''\right)}} \tag{10}$$

note

$$\epsilon' + \epsilon'' = t - t' + t' - t'' = t - t'' \tag{11}$$

so

$$U_0\left(x, x''; t, t''\right) = \sqrt{\frac{m}{2\pi\imath\hbar\left(t-t''\right)}} e^{\frac{\imath m\left(x-x''\right)^2}{2\hbar\left(t-t''\right)}} \tag{12}$$

By successively performing such Gaussian integrals

$$U_0\left(x, x'; t, 0\right) = \sqrt{\frac{m}{2\pi\imath\hbar t}} e^{\frac{\imath m\left(x-x''\right)^2}{2\hbar t}} \tag{13}$$

# 2 Problem 2

In three dimension the Hamiltonian for two interacting particle is

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V\left(\vec{r}_1 - \vec{r}_2\right) \tag{14}$$

## 2.1 a: Transforming to CM coordinates

We define from classical mechanics the CM

$$\vec{R}_{CM} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2} \tag{15}$$

and

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \tag{16}$$

we can rewrite $\vec{r}_1$ and $\vec{r}_2$

$$\vec{r}_1 = \vec{R}_{CM} + \frac{m_2}{m_1+m_2}\vec{r} \tag{17}$$

$$\vec{r}_2 = \vec{R}_{CM} - \frac{m_1}{m_1+m_2}\vec{r} \tag{18}$$

define

$$\vec{p}_{CM} \equiv \underbrace{(m_1 + m_2)}_{M} \dot{\vec{R}}_{CM} \tag{19}$$

$$\vec{p} \equiv \frac{m_1 m_2}{m_1 + m_2} \dot{\vec{r}} \tag{20}$$

note that

$$\vec{p}_i = \frac{m_i}{M} \vec{p}_{CM} + (-1)^i \vec{p} \tag{21}$$

The Hamiltonian in our new coordinates

$$H = \frac{1}{2m_1} \left( \frac{m_1}{M} \vec{p}_{CM} + \vec{p} \right)^2 + \frac{1}{2m_2} \left( \frac{m_2}{M} \vec{p}_{CM} - \vec{p} \right)^2 + V(r) \tag{22}$$

$$= \frac{1}{2} \left( \frac{m_1}{M^2} + \frac{m_2}{M^2} \right) p_{CM}^2 + \frac{1}{2} \left( \frac{1}{m_1} + \frac{1}{m_2} \right) p^2 + V(\vec{r}) \tag{23}$$

$$H = \underbrace{\frac{p_{CM}^2}{2M}}_{H_{CM}} + \underbrace{\frac{p^2}{2\mu} + V(\vec{r})}_{H_{rel}} \tag{24}$$

where

$$M \equiv m_1 + m_2 \tag{25}$$

$$\mu \equiv \frac{m_1 m_2}{m_1 + m_2} \tag{26}$$

## 2.2 b: Commutation relations

$$\left[ R_{CM}^i, p_{CM}^j \right] = \left[ \frac{m_1}{M} r_1^i, p_1^j \right] + \left[ \frac{m_2}{M} r_2^j, p_2^j \right] \tag{27}$$

$$\left[ R_{CM}^i, p_{CM}^j \right] = \imath\hbar\delta_{ij} \tag{28}$$

$$\left[ R_{CM}^i, p^j \right] = \left[ \frac{m_1}{M} r_1^i, \frac{m_2}{M} p_1^j \right] - \left[ \frac{m_2}{M} r_2^i, \frac{m_1}{M} p_2^j \right] \tag{29}$$

$$\left[ R_{CM}^i, p^j \right] = 0 \tag{30}$$

$$\left[ r^i, p_{CM}^j \right] = \left[ r_1^i, p_1^j \right] - \left[ r_2^i, p_2^j \right] \tag{31}$$

$$\left[ r^i, p_{CM}^j \right] = 0 \tag{32}$$

$$\left[ r^i, p^j \right] = \underbrace{\left[ r_1^i, \frac{m_2}{M} p_1^j \right]}_{\frac{m_2}{M} \imath\hbar\delta_{ij}} + \underbrace{\left[ r_2^i, \frac{m_1}{M} p_2^j \right]}_{\frac{m_1}{M} \imath\hbar\delta_{ij}} \tag{33}$$

$$\left[ r^i, p^j \right] = \imath\hbar\delta_{ij} \tag{34}$$

## 2.3 c: Separable solutions

we know from the form of $H$ that the eigenstates are separable

$$\Psi\left(R_{CM}, r\right) = \psi_{CM}\left(R_{CM}\right) \times \psi_{r}\left(r\right) \tag{35}$$

using the above we can write the Hamiltonian in a more convenient form

$$H\Psi = E\Psi \tag{36}$$
$$\left(H_{CM}\psi_{CM}\right)\psi_{rel} + \psi_{CM}\left(H_{rel}\psi_{rel}\right) = E\psi_{CM}\psi rel \tag{37}$$

which give us two independent equations

$$H_{CM}\psi_{CM} = E_{CM}\psi_{CM} \tag{38}$$
$$H_{rel}\psi_{rel} = E_{rel}\psi_{rel} \tag{39}$$

with

$$E = E_{CM} + E_{rel} \tag{40}$$

because the $CM$ Hamiltonian has no potential the solutions are just plane waves

$$\psi_{CM}\left(R_{CM}\right) = e^{\imath\vec{k}_{CM}\cdot\vec{R}_{CM}} \tag{41}$$
$$E_{CM} = \frac{\hbar^2 k_{CM}^2}{2M} \tag{42}$$

## 2.4 d: $Y_l^m$'s are separable

For the $\psi_{rel}$ we note that Hamiltonian is invariant under rotations which means that energy eigen states are also eigen states of the angular momentum operator $L^2$.

$$H\psi_{rel} = \left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right) + \frac{L^2}{2\mu r^2} + V\left(r\right)\right]\psi_{rel} \tag{43}$$

$\psi_{rel}$ is separable.

$$\psi_{rel}\left(r,\theta,\phi\right) = R\left(r\right)Y_\ell^m\left(\theta,\phi\right) \tag{44}$$

where

$$L^2 Y_\ell^m\left(\theta,\phi\right) = \ell\left(\ell+1\right)\hbar^2 Y_\ell^m\left(\theta,\phi\right) \tag{45}$$
$$L_z Y_\ell^m\left(\theta,\phi\right) = \hbar m Y_\ell^m\left(\theta,\phi\right) \tag{46}$$

plugging this into the S.E.

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right)R + \left(V\left(r\right) + \frac{\ell\left(\ell+1\right)\hbar^2}{2\mu r^2}\right)R = ER \tag{47}$$

These $Y_\ell^m$'s are separable

$$Y_\ell^m\left(\theta,\phi\right) = \Theta_\ell^m\left(\theta\right)\Phi^m\left(\phi\right) \tag{48}$$

the angular part of the differential equation becomes.

$$\left[\frac{-1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}m^2\right]\Theta_\ell^m(\theta)=\ell(\ell+1)\hbar^2\Theta_\ell^m(\theta) \tag{49}$$

$$-\frac{\partial^2}{\partial\phi^2}\Phi^m(\phi)=m^2\Phi^m(\phi) \tag{50}$$

$$\Phi(\phi)=e^{\imath m\phi},\text{ where } m\in\mathbb{Z} \tag{51}$$

# 3 Problem 3

Suppose we have 3 bosons in a box measured to have states $n=3$, $n=3$, and $n=4$. We can build the wave function from the single state wave functions

$$\psi_n(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) \tag{52}$$

by first finding the product wave function

$$\Psi_{n_1n_2n_3}^{(product)}(x_1,x_2,x_3)=\left(\frac{2}{L}\right)^{\frac{3}{2}}\sin\left(\frac{n_1\pi}{L}x_1\right)\sin\left(\frac{n_2\pi}{L}x_2\right)\sin\left(\frac{n_3\pi}{L}x_3\right) \tag{53}$$

and then symmetrizing

$$\begin{aligned}\Psi_{n_1n_2n_3}(x_1,x_2,x_3)=\sqrt{\frac{1}{3!}}\Big[&\Psi_{n_1n_2n_3}^{(product)}(x_1,x_2,x_3)+\Psi_{n_1n_2n_3}^{(product)}(x_2,x_3,x_1)\\&+\Psi_{n_1n_2n_3}^{(product)}(x_3,x_1,x_2)+\Psi_{n_1n_2n_3}^{(product)}(x_3,x_2,x_1)\\&+\Psi_{n_1n_2n_3}^{(product)}(x_2,x_1,x_3)+\Psi_{n_1n_2n_3}^{(product)}(x_1,x_3,x_2)\Big].\end{aligned} \tag{54}$$

These wave function don't change at all under the exchange of the two $n=3$ particle which means that this sum of six wave functions can be simplified to a sum of three wave functions

$$\begin{aligned}\Psi_{n_1n_2n_3}(x_1,x_2,x_3)=\frac{1}{\sqrt{3}}\left(\frac{2}{L}\right)^{3/2}\Big[&\sin\frac{n\pi}{L}x_1\sin\frac{n\pi}{L}x_2\sin\frac{m\pi}{L}x_3+\\&\sin\frac{n\pi}{L}x_2\sin\frac{n\pi}{L}x_3\sin\frac{m\pi}{L}x_1+\sin\frac{n\pi}{L}x_3\sin\frac{n\pi}{L}x_1\sin\frac{m\pi}{L}x_2\Big],\end{aligned} \tag{55}$$

with $n=3$ and $m=4$.

# 4 Problem 4

## 4.1 a: Distinguishable

Each particle has a choice of three states which is

$$3*3*3=27 \tag{56}$$

total

## 4.2 b: Identical bosons

There are no restriction on the number of particle allow in each states. I prefer to visualize this as an Einstein solid. Here are a few examples of configurations
one particle in each state

$$0|0|0 \tag{57}$$

two particles in $a$ and one particle in $c$

$$0\,0|\,|0 \tag{58}$$

all three particles in $b$

$$|0\,0\,0| \tag{59}$$

The number of independent combinations is

$$\frac{\left(N_{|} + N_0\right)!}{N_{|}!N_0!} = \frac{(2+3)!}{2!3!} = 10 \tag{60}$$

## 4.3 c: Identical fermions

cells can hold either no particle or one particle, the only possibility is one in each state.

# 5 Problem 5

## 5.1 a: Translation operator

The transformation for $H$ is

$$T_{\epsilon}^{\dagger} H T_{\epsilon} = \frac{p^2}{2m} + V\left(x + \epsilon\right) \tag{61}$$

$H$ is only invariant if $\epsilon = na$, where $n \in \mathbb{Z}$. Therefore,

$$[T_{na}, H] = 0, \text{ if } n \in \mathbb{Z} \tag{62}$$

## 5.2 b: Bloch states

$T$ is unitary so it can be put in the form.

$$T = e^{\frac{\imath a}{\hbar} p} \tag{63}$$

Where $p^{\dagger} = p$. We use $p$ here because for the translation this quantity turns out to be the momentum operator, but as a general statement this should just be some hermitian operator. From part 'a' we know that eigenstates of $H$ are also eigenstates of $T_{na}$. Because $T$ is unitary it's eigenvalues must be

$$|\lambda_k| = 1 \tag{64}$$

ie.

$$\lambda_k = e^{\imath ka} \tag{65}$$

so

$$T_a \psi_k (x) = e^{\imath ka} \psi_k (x) = \psi_k (x + a) \tag{66}$$

so

$$\psi_{k,n} (x) = e^{\imath kx} u_{k,n} (x), \text{ where } u_{k,n} (x) = u_{k,n} (x + a) \tag{67}$$

This is know as Bloch's Theorem.

### 5.3 c: S.E. for Bloch waves

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \left( e^{\imath kx} u_{k,n} (x) \right) + V (x) e^{\imath kx} u_{k,n} (x) = E_n (k) e^{\imath kx} u_{k,n} (x) \tag{68}$$

taking the derivative, where k is just a parameter

$$-\frac{\hbar^2}{2m} \partial_x^2 u_{k,n} (x) - \imath \frac{\hbar^2 k}{m} \partial_x u_{k,n} (x) + \left( \frac{\hbar^2 k^2}{2m} + V (x) \right) u_{k,n} (x) = E_n (k) u_{k,n} (x) \tag{69}$$

A nice way to get the above result is by using the relation below

$$\left[ p^2, f (x) \right] = p [p, f] + [p, f] p = -\hbar^2 \partial_x^2 f - 2\imath\hbar \partial_x f p \tag{70}$$

### 5.4 d: Eigenvalue properties

note that

$$\psi_{k,n} (x) = e^{\imath kx} u_{k,n} (x) \tag{71}$$

for outside the range $0 < k < \frac{2\pi}{a}$, a.k.a the first Brillouin zone

$$k = \frac{2\pi}{a} n + k', \text{ where } n \in \mathbb{Z} \text{ and } 0 < k' < \frac{2\pi}{a} \tag{72}$$

$$\psi_{k,n} (x) = e^{\imath k' x} \underbrace{e^{\imath \frac{2\pi}{a} nx} u_{k,n} (x)}_{\equiv u_{k'} (x)} \tag{73}$$

It is clear from this and from Eq.67 that there is no physical distinction between states with eigenvalues $k$ and $k + s2\pi/a$ ($s$ an integer) and thus the eigenvalue of the $u_{k,n}(x)$ must be periodic in $k$ with period $2\pi/a$, i.e., $E_n(k) = E_n(k + 2\pi/a)$. This should also be clear from direct examination of Eq.69 for a periodic $V(x)$, particularly after Fourier-transforming the equation.

## 6 Problem 6

Compute The ground state for N-particles in a box of size $L$ when the particles are identical, spin-polarized.

## 6.1 a: Bosons

all of the particles can go into the ground state of a single particle. so the many particle ground state energy is

$$E_{gs}^{(Bosons)} = \sum_{i=1}^{N} E_1 = N \frac{\hbar^2 \pi^2}{2mL^2} \tag{74}$$

## 6.2 b: Fermions

There can only be one fermion per state so the ground state energy is

$$E_{gs}^{(fermions)} = \sum_{n=1}^{N} E_n = \frac{\hbar^2 \pi^2}{2mL^2} \underbrace{\sum_{n=1}^{N} n^2}_{\approx \int_0^N dn n^2 = \frac{N^3}{3}} \tag{75}$$

$$E_{gs}^{(fermions)} = \frac{\hbar^2 \pi^2}{6mL^2} N^3 \tag{76}$$