Prof. Dr. Viatcheslav Mukhanov Winter term 2019/2020

Exercises on Quantum Mechanics II (TM1/TV)

Problem set 10, discussed January 7 - January 10, 2019

Exercise 58 - Short questions

(i) Name at least four physical effects which can be explained with quantum mechanics and not with classical mechanics.

(ii) Suppose you are given a Hamiltonian of a free particle. What are the main things you should do in order to quantize the system?

(iii) Which of the following operators are Hermitian? Position operator, momentum operator, annihilation operator (defined in the analysis of harmonic oscillator), Hamiltonian. Give another example of a non-Hermitian operator.

(iv) Simplify the following expression

$$[\hat{p}\hat{q}, \hat{q}^2] \tag{1}$$

(v) What property does an operator have to satisfy to correspond to a physical observable? Why?

(vi) Give an example of compatible operators (i.e. those who's commutator vanishes). What does this imply for the eigenvectors of the operators if the operators have non-degenerate eigenvalues? Why?

(vii) Show that the hermicity of Hamilton operator follows from the unitarity of the time-evolution operator.

(viii) Consider a system of two pendulums of length l on whose ends are attached balls of mass m. Suppose that these two balls are connected via weak spring k. (Figure 1.) The Lagrangian of the system is then given by

$$L = \frac{1}{2}ml^2\dot{\theta}_1^2 + \frac{1}{2}ml^2\dot{\theta}_2^2 - \frac{1}{2}mgl\theta_1^2 - \frac{1}{2}mgl\theta_2^2 - \frac{1}{2}kl^2(\theta_2 - \theta_1)^2 \tag{2}$$

Find the normal coordinates in terms of θ_1 and θ_2. What is the spectrum of the Hamiltonian after quantization?

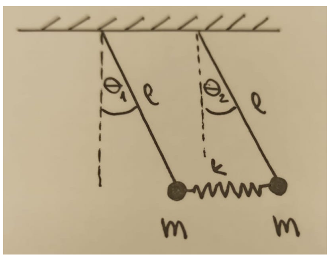

Figure 1: Pendulums connected via spring.

(ix) Suppose we have 2 systems which in the beginning do not interact. Then they interact and at some point stop interacting again. Can we write the wave function of the full system as a product of wave functions of first and second system after they stop interacting?

(x) Consider a particle in a potential $\hat{V}$. How can you interpret the zeroth, first and second order of the perturbation expansion of the propagator $K(f, i)$? Write them down.

Solutions

(i) Black body radiation, Photoelectric effect, Hydrogen atom, Stern Gerlach experiment...

(ii) Put hats and postulate canonical commutation relations.

(iii) All but annihilation operator.

(iv)
$$[\hat{p}\hat{q}, \hat{q}^2] = [\hat{p}, \hat{q}^2]\hat{q} = -2i\hbar\hat{q}^2 \tag{3}$$

(v) It has to be hermitian because then it's eigenvalues are real.

(vi) Hamiltonian and number operator of harmonic oscillator are commuting. They have common eigenvectors. One more example would be the commutator $\left[L_x, L^2\right] = 0$ where L is angular momentum operator. For the derivation of this result see exercize 22.

(vii) exercise 35

(viii) The angles in the Lagrangian are clearly coupled. In order to describe the system in an easier way it is therefore convenient to introduce normal coordinates which decouple the system into two harmonic oscillators. By observing the Lagrangian, one can easily see that this can be done by defining

$$\zeta_1 = \frac{1}{\sqrt{2}}(\theta_1 + \theta_2) \qquad \zeta_2 = \frac{1}{\sqrt{2}}(\theta_1 - \theta_2) \tag{4}$$

Substituting this in the Lagrangian we obtain

$$L = \frac{1}{2}ml^2\dot{\zeta}_1^2 + \frac{1}{2}ml^2\dot{\zeta}_2^2 - \frac{1}{2}mgl\zeta_1^2 - \frac{1}{2}mgl\zeta_2^2 - kl^2\zeta_2^2 \tag{5}$$

Clearly, we now have a system of two decoupled harmonic oscillators. It is convenient to normalize the coordinates such that in front of the velocities we have just a factor of $\frac{1}{2}$. Defining

$$\tilde{\zeta}_1 = \sqrt{m}l\zeta_1 \qquad \tilde{\zeta}_2 = \sqrt{m}l\zeta_2 \tag{6}$$

we obtain a system represented by two harmonic oscillators

$$L = \frac{1}{2}\dot{\tilde{\zeta}}_1^2 - \frac{1}{2}\omega_1^2\tilde{\zeta}_1^2 + \frac{1}{2}\dot{\tilde{\zeta}}_2^2 - \frac{1}{2}\omega_2^2\tilde{\zeta}_2^2 \tag{7}$$

with frequencies $\omega_1 = \sqrt{\frac{g}{l}}$ and $\omega_2 = \sqrt{\frac{g}{l} + \frac{2k}{m}}$.
From here, one can easily see following the analysis similar to a one dimensional harmonic oscillator, that the energy spectrum corresponding to this system is given by

$$\begin{aligned} E_{n_1,n_2} &= E_{n_1} + E_{n_2} \\ E_{n_1} &= \hbar\omega_1(n_1 + \frac{1}{2}) \qquad E_{n_2} = \hbar\omega_2(n_2 + \frac{1}{2}) \end{aligned} \tag{8}$$

(ix) No, because we have an entangled state.

(x) In the Problem sheet 8, ex. 48 we have derived the following expressions which we can interpret as

$$\begin{aligned} K(f,i) &= K_0(f,i) + K_1(f,i) + K_2(f,i) + ... \\ K_0(f,i) &= \int_{q_i}^{q_f} \mathcal{D}q e^{\frac{i}{\hbar}S_0} \\ K_1(f,i) &= -\frac{i}{\hbar}\int_{t_i}^{t_f} dt_I \int dq_I K_0(f,I)V(I)K_0(I,i) \\ K_2(f,i) &= -\frac{1}{\hbar^2}\int_{t_i}^{t_f} dt_{II} \int_{t_i}^{t_{II}} dt_I \int dq_{II} \int dq_I K_0(f,II)V(II)K_0(II,I)V(I)K_0(I,i) \end{aligned} \tag{9}$$

We can interpret zeroth order $K_0(f,i)$ as no scattering between particle and potential, because this is just the propagator of a free particle from initial to final state. The first correction can be interpreted as following - the particle freely moves until it scatters one time with the potential. After this it moves freely until final state. Finally, the second correction, $K_2(f,i)$ we can interpret as particle scattering of a potential two times.

Exercise 59 - Quantization

Consider a classical scalar field theory with the Lagrangian density (we are using the mostly minus metric)

$$\mathcal{L} = \frac{1}{2}\left(\partial_\mu\phi\partial_\nu\phi\eta^{\mu\nu} - m^2\phi^2\right). \tag{10}$$

(i) Find the conjugate momenta and the Hamiltonian density.

(ii) Find the equation of motion and by Fourier expanding the field as

$$\phi(t,\boldsymbol{x}) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\boldsymbol{k}.\boldsymbol{x}}\phi_{\boldsymbol{k}}(t), \tag{11}$$

show that the dispersion relation is $\omega_k^2 = \boldsymbol{k}^2 + m^2$. What property does $\phi_{\boldsymbol{k}}(t)$ have under complex conjugation?

We can define the equal time Poisson bracket for two functionals f and g as

$$\{f(t,\boldsymbol{x}), g(t,\boldsymbol{y})\} = \int d^3z \left(\frac{\delta f(t,\boldsymbol{x})}{\delta\phi(t,\boldsymbol{z})}\frac{\delta g(t,\boldsymbol{y})}{\delta\pi(t,\boldsymbol{z})} - \frac{\delta g(t,\boldsymbol{y})}{\delta\phi(t,\boldsymbol{z})}\frac{\delta f(t,\boldsymbol{x})}{\delta\pi(t,\boldsymbol{z})}\right). \tag{12}$$

(iii) Find the equal time Poisson brackets of all combinations of ϕ and π.

(iv) We can define

$$a_{\boldsymbol{k}}(t) = \int \frac{d^3x}{(2\pi)^{3/2}} a(\boldsymbol{x})e^{-i\boldsymbol{k}.\boldsymbol{x}} = \int \frac{d^3x}{(2\pi)^{3/2}} e^{-i\boldsymbol{k}.\boldsymbol{x}}\sqrt{\frac{\omega_k}{2}}\left(\phi(t,\boldsymbol{x}) + \frac{i}{\omega_k}\pi(t,\boldsymbol{x})\right) \tag{13}$$

and the corresponding complex conjugate $a^*_{\boldsymbol{k}}(t)$. Use your result of the previous question to find the equal time Poisson brackets of all combinations of $a_{\boldsymbol{k}}(t)$ and $a^*_{\boldsymbol{k}}(t)$.

(v) Find the equations of motion of $a_{\boldsymbol{k}}(t)$ and $a^*_{\boldsymbol{k}}(t)$ and show that

$$a_{\boldsymbol{k}}(t) = a_{\boldsymbol{k}}e^{-i\omega_k t} \quad \text{and} \quad a^*_{\boldsymbol{k}}(t) = a^*_{\boldsymbol{k}}e^{i\omega_k t} \tag{14}$$

Use this to show that we can write the field as

$$\begin{aligned}\phi(t,\boldsymbol{x}) &= \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}}\left(a_{\boldsymbol{k}}(t)e^{i\boldsymbol{k}.\boldsymbol{x}} + a_{\boldsymbol{k}}(t)^*e^{-i\boldsymbol{k}.\boldsymbol{x}}\right) \\ &= \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}}\left(a_{\boldsymbol{k}}e^{-ik.x} + a^*_{\boldsymbol{k}}e^{ik.x}\right),\end{aligned} \tag{15}$$

where $k.x = \omega t - \boldsymbol{k}.\boldsymbol{x}$.

(vi) So far everything has been done classically. What do we have to do to move to the quantum picture? Write down all the Poisson brackets you calculated in the quantum picture. What is different?

(vii) Show that the Heisenberg equation reproduces the equations of motion of the classical system for ϕ and π in the quantum mechanical picture.

Solution

(i) By definition the canonical momentum is

$$\pi(t,\boldsymbol{x}) = \frac{\partial\mathcal{L}}{\partial\dot{\phi}(t,\boldsymbol{x})} = \dot{\phi}(t,\boldsymbol{x}). \tag{16}$$

and the Hamiltonian density,

$$\mathcal{H} = \frac{1}{2}\left(\pi^2 - \partial_i\phi\partial^i\phi + m^2\phi^2\right). \tag{17}$$

(ii) Either by directly using

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} - \frac{\partial \mathcal{L}}{\partial \phi} = 0 \tag{18}$$

or using

$$\partial_t \pi = -\frac{\partial \mathcal{H}}{\partial \phi} + \partial_i \frac{\partial \mathcal{H}}{\partial(\partial_i \phi)} \tag{19}$$

we find the equation of motion

$$\partial_\mu \partial^\mu \phi + m^2 \phi = 0 \tag{20}$$

By applying the equation of motion to the Fourier expansion,

$$\frac{\mathrm{d}^2 \phi_{\boldsymbol{k}}}{\mathrm{d}t^2} + (\boldsymbol{k}^2 + m^2)\phi_{\boldsymbol{k}} = 0, \tag{21}$$

which is the equation of motion of the harmonic oscillator with dispersion relation

$$\omega_k = \sqrt{\boldsymbol{k}^2 + m^2}. \tag{22}$$

As the field $\phi(t, \boldsymbol{x})$ is real we see from the Fourier decomposition that $\phi^*_{\boldsymbol{k}} = \phi_{-\boldsymbol{k}}$.

(iii) Using the definition of the Poisson bracket,

$$\begin{aligned}
\{\phi(t, \boldsymbol{x}), \pi(t, \boldsymbol{y})\} &= \int d^3 z \delta^3(\boldsymbol{x} - \boldsymbol{z})\delta^3(\boldsymbol{y} - \boldsymbol{z}) = \delta^3(\boldsymbol{x} - \boldsymbol{y}) \\
\{\phi(t, \boldsymbol{x}), \phi(t, \boldsymbol{y})\} &= \{\pi(t, \boldsymbol{x}), \pi(t, \boldsymbol{y})\} = 0.
\end{aligned} \tag{23}$$

(iv) We can use the result of the previous question to find

$$\begin{aligned}
\{a_{\boldsymbol{k}}(t), a^*_{\boldsymbol{p}}(t)\} &= \int \frac{d^3 x}{(2\pi)^{3/2}} \frac{d^3 y}{(2\pi)^{3/2}} e^{-i\boldsymbol{k}.\boldsymbol{x}} e^{+i\boldsymbol{p}.\boldsymbol{y}} \sqrt{\frac{\omega_k \omega_p}{4}} \left[\frac{i}{\omega_k}\{\pi(t, \boldsymbol{x}), \phi(t, \boldsymbol{y})\} - \frac{i}{\omega_p}\{\phi(t, \boldsymbol{x}), \pi(t, \boldsymbol{y})\}\right] \\
&= \int \frac{d^3 x}{(2\pi)^{3/2}} \frac{d^3 y}{(2\pi)^{3/2}} e^{-i\boldsymbol{k}.\boldsymbol{x}} e^{+i\boldsymbol{p}.\boldsymbol{y}} \sqrt{\frac{\omega_k \omega_p}{4}} \left[-\frac{i}{\omega_k} - \frac{i}{\omega_p}\right] \delta^3(\boldsymbol{x} - \boldsymbol{y}) \\
&= \int \frac{d^3 x}{(2\pi)^3} e^{-i(\boldsymbol{k}-\boldsymbol{p}).\boldsymbol{x}} \sqrt{\frac{\omega_k \omega_p}{4}} \left[-\frac{i}{\omega_k} - \frac{i}{\omega_p}\right] \\
&= -i\delta^3(\boldsymbol{k} - \boldsymbol{p}).
\end{aligned} \tag{24}$$

Similarly,

$$\{a_{\boldsymbol{k}}(t), a_{\boldsymbol{p}}(t)\} = \{a^*_{\boldsymbol{k}}(t), a^*_{\boldsymbol{p}}(t)\} = 0. \tag{25}$$

(v) The equation of motion is given by

$$\begin{aligned}
\dot{a}_{\boldsymbol{k}}(t) &= -\{H, a_{\boldsymbol{k}}(t)\} \\
&= -\int \frac{d^3 x}{(2\pi)^{3/2}} e^{-i\boldsymbol{k}.\boldsymbol{x}} \sqrt{\frac{\omega_k}{2}} \left(\{H, \phi(t, \boldsymbol{x})\} + \frac{i}{\omega_k}\{H, \pi(t, \boldsymbol{x})\}\right),
\end{aligned} \tag{26}$$

where

$$\begin{aligned}
\{H, \phi(t, \boldsymbol{x})\} &= -\pi(t, \boldsymbol{x}), \\
\{H, \pi(t, \boldsymbol{x})\} &= \int d^3 z \; \delta^3(\boldsymbol{x} - \boldsymbol{z}) \frac{\delta H}{\delta \phi(t, \boldsymbol{z})} \\
&= \int d^3 y \delta^3(\boldsymbol{x} - \boldsymbol{y})(-\Delta + m^2)\phi(t, \boldsymbol{y}) \\
&= (\boldsymbol{k}^2 + m^2)\phi(t, \boldsymbol{x}) \\
&= \omega_k^2 \phi(t, \boldsymbol{x})
\end{aligned} \tag{27}$$

Hence we have

$$\begin{aligned}
\dot{a}_{\boldsymbol{k}}(t) &= -\int \frac{d^3 x}{(2\pi)^{3/2}} e^{-i\boldsymbol{k}.\boldsymbol{x}} \sqrt{\frac{\omega_k}{2}} \left(-\pi(t, \boldsymbol{x}) + i\omega_k \phi(t, \boldsymbol{x})\right) \\
&= -i\omega_k a_{\boldsymbol{k}}(t),
\end{aligned} \tag{28}$$

which is easily solved to give the solutions stated in the question.

By substitution we can show

$$
\begin{aligned}
\phi(t,\boldsymbol{x}) &= \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}} \left(a_{\boldsymbol{k}}(t)e^{i\boldsymbol{k}.\boldsymbol{x}} + a_{\boldsymbol{k}}(t)^* e^{-i\boldsymbol{k}.\boldsymbol{x}}\right) \\
&= \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}} \frac{d^3y}{(2\pi)^{3/2}} \sqrt{\frac{\omega_k}{2}} \\
&\times \left[e^{i\boldsymbol{k}.(\boldsymbol{x}-\boldsymbol{y})}\left(\phi(t,\boldsymbol{y}) + \frac{i}{\omega_k}\pi(t,\boldsymbol{y})\right) + e^{-i\boldsymbol{k}.(\boldsymbol{x}-\boldsymbol{y})}\left(\phi(t,\boldsymbol{y}) - \frac{i}{\omega_k}\pi(t,\boldsymbol{y})\right)\right] \\
&= \int d^3y\ \delta^3(\boldsymbol{x}-\boldsymbol{y})\phi(t,\boldsymbol{y}) \\
&= \phi(t,\boldsymbol{x}).
\end{aligned} \tag{29}
$$

(vi) We have basically done all the work, we can move to the quantum picture simply by promoting ϕ and π to operators and replacing the Poisson bracket with the commutator,

$$
\begin{aligned}
\phi(t,\boldsymbol{x}) &\to \hat{\phi}(t,\boldsymbol{x}) \\
\pi(t,\boldsymbol{x}) &\to \hat{\pi}(t,\boldsymbol{x}) \\
\{\ .\ ,\ .\ \} &\to -i[\ .\ ,\ .\ ].
\end{aligned} \tag{30}
$$

The commutators in of the field operator and the conjugate momentum become

$$
\begin{aligned}
\left[\hat{\phi}(t,\boldsymbol{x}), \hat{\pi}(t,\boldsymbol{y})\right] &= i\delta^3(\boldsymbol{x}-\boldsymbol{y}) \\
\left[\hat{\phi}(t,\boldsymbol{x}), \hat{\phi}(t,\boldsymbol{y})\right] &= [\hat{\pi}(t,\boldsymbol{x}), \hat{\pi}(t,\boldsymbol{y})] = 0.
\end{aligned} \tag{31}
$$

And the commutators of the Fourier operators become

$$
\begin{aligned}
\left[\hat{a}_{\boldsymbol{k}}(t), \hat{a}^\dagger_{\boldsymbol{p}}(t))\right] &= \delta^3(\boldsymbol{k}-\boldsymbol{p}) \\
[\hat{a}_{\boldsymbol{k}}(t), \hat{a}_{\boldsymbol{p}}(t)] &= \left[\hat{a}^\dagger_{\boldsymbol{k}}(t), \hat{a}^\dagger_{\boldsymbol{p}}(t)\right] = 0.
\end{aligned} \tag{32}
$$

(vii) Starting from the Heisenberg equation of motion, with the quatized Eq. 17, for $\hat{\pi}$,

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\hat{\phi}(t,\boldsymbol{x}) &= i\left[\int d^3y\ \hat{\mathcal{H}}(t,\boldsymbol{y}), \hat{\phi}(t,\boldsymbol{x})\right] \\
&= i\int d^3y\ \left[\frac{1}{2}\left(\hat{\pi}^2 - \partial_i\hat{\phi}\partial^i\hat{\phi} + m^2\hat{\phi}^2\right)(t,\boldsymbol{y}), \hat{\phi}(t,\boldsymbol{x})\right] \\
&= \frac{i}{2}\int d^3y\ \left[\hat{\pi}^2(t,\boldsymbol{y}), \hat{\phi}(t,\boldsymbol{x})\right] \\
&= i\int d^3y\ \left[\hat{\pi}(t,\boldsymbol{y}), \hat{\phi}(t,\boldsymbol{x})\right]\hat{\pi}(t,\boldsymbol{y}) \\
&= i\int d^3y\ \left(-i\delta^3(\boldsymbol{x}-\boldsymbol{y})\right)\hat{\pi}(t,\boldsymbol{y}) \\
&= \hat{\pi}(t,\boldsymbol{x}).
\end{aligned} \tag{33}
$$

And similarly for $\hat{\pi}$,

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\hat{\pi}(t,\boldsymbol{x}) &= i\left[\int d^3y\ \hat{\mathcal{H}}(t,\boldsymbol{y}), \hat{\pi}(t,\boldsymbol{x})\right] \\
&= i\int d^3y\ \left[\frac{1}{2}\left(\hat{\pi}^2 - \partial_i\hat{\phi}\partial^i\hat{\phi} + m^2\hat{\phi}^2\right)(t,\boldsymbol{y}), \hat{\pi}(t,\boldsymbol{x})\right] \\
&= \frac{i}{2}\int d^3y\ \left[\left(-\partial_i\hat{\phi}\partial^i\hat{\phi} + m^2\hat{\phi}^2\right)(t,\boldsymbol{y}), \hat{\pi}(t,\boldsymbol{x})\right] \\
&= i\int d^3y\ \left(-\partial_{(\boldsymbol{y}),i}\hat{\phi}(t,\boldsymbol{y})\ \partial^i_{(\boldsymbol{y})}\left[\hat{\phi}(t,\boldsymbol{y}), \hat{\pi}(t,\boldsymbol{x})\right] + m^2\hat{\phi}(t,\boldsymbol{y})\left[\hat{\phi}(t,\boldsymbol{y}), \hat{\pi}(t,\boldsymbol{x})\right]\right) \\
&= i\int d^3y\ \left(-\partial_{(\boldsymbol{y}),i}\hat{\phi}(t,\boldsymbol{y})\ \partial^i_{(\boldsymbol{y})}(i\delta^3(\boldsymbol{x}-\boldsymbol{y})) + m^2\hat{\phi}(t,\boldsymbol{y})i\delta^3(\boldsymbol{x}-\boldsymbol{y})\right) \\
&= -\partial_i\partial^i\hat{\phi}(t,\boldsymbol{x}) - m^2\hat{\phi}(t,\boldsymbol{x}) \\
&\implies \partial_\mu\partial^\mu\hat{\phi} + m^2\hat{\phi} = 0.
\end{aligned} \tag{34}
$$

Exercise 60 - Density matrix in 2-dimensions and Bloch Sphere

We are going to discuss the density matrix formalism in the case of a 2-dimensional Hilbert space; as a physical example, it corresponds to the Hilbert space of a spin 1/2 particle.

(i) First of all, let's see how a state looks like. Prove that a generic normalized state (i.e. a ray-vector of the Hilbert space) can be written as

$$|\,\psi\rangle = \cos\left(\frac{\theta}{2}\right)|\,0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|\,1\rangle \quad \text{with} \quad \theta\in[0,\pi] \quad , \quad \phi\in[0,2\pi] \tag{35}$$

where $|\,0\rangle\,,|\,1\rangle$ are the eigenvectors of the Pauli matrix $\hat{\sigma}_3$ (the choice of $\hat{\sigma}_3$ is purely conventional). Show that this means that the 2-dimensional Hilbert space of normalized states is isomorphic to the 2-Sphere S^2. In this geometric picture every state $|\,\psi\rangle$ is a point of S^2: in this context, the sphere is called **Bloch Sphere**.

(ii) Let's try now to enlarge our view considering also mixed states. To do that, we want to study first how a general density matrix looks like. Recalling that $\{\mathbb{1},\boldsymbol{\sigma}\}$ (where $\boldsymbol{\sigma}=(\hat{\sigma}_1,\hat{\sigma}_2,\hat{\sigma}_3)$) form a basis for the operators in a 2-dimensional Hilbert space, it means that the most general operator is of the form:

$$\hat{\rho}_{\alpha,\boldsymbol{\beta}} = \alpha\mathbb{1} + \boldsymbol{\beta}\cdot\boldsymbol{\sigma} \tag{36}$$

Recalling the properties of a density matrix, find conditions on $\alpha,\boldsymbol{\beta}$ to make $\hat{\rho}$ a density matrix.

You should find:

$$\hat{\rho}_{\boldsymbol{r}} = \frac{1}{2}(\mathbb{1}+\boldsymbol{r}\cdot\boldsymbol{\sigma}) \quad \text{with} \quad |\boldsymbol{r}|\le 1 \quad \boldsymbol{r}\in\mathbb{R}^3 \tag{37}$$

Therefore, all states (pure and mixed) live within the interior of the Bloch Sphere.

(iii) For which $\boldsymbol{r}$ does $\hat{\rho}$ represent a pure state? And a mixed one? Would you expect this from what you had found in part (i)?

(iv) Show that two orthonormal vectors are located at antipodal points on the Bloch sphere.

(v) Consider the Hamilton operator $\hat{H}=a\boldsymbol{B}\cdot\boldsymbol{\sigma}$. Compute its expectation value in the state given by $\hat{\rho}_{\boldsymbol{r}}$.

(vi) For which value of $\boldsymbol{r}$ does $\hat{\rho}_{\boldsymbol{r}}$ correspond to a spin one-half particle which is randomly produced with probability 1/2 in the state $|\,0\rangle$ and with probability 1/2 in the state $|\,1\rangle$? What is the the entropy in this case?

(vii) A density matrix is said to be describing a maximally entangled state if it has maximum entanglement entropy (or Von Neuman entropy). What is the maximum entanglement entropy in this case? To which $\boldsymbol{r}$ (i.e. which point(s) in the Bloch Sphere) does it correspond?

(viii) Consider now spin one-half particles which are produced with spins in any direction with equal probability. Calculate the density matrix.

Solution

(i) Since $\{|\,0\rangle\,,|\,1\rangle\}$ is an orthonormal basis for the Hilbert space, a generic normalized state is of the form:

$$|\,\psi\rangle = a\,|\,0\rangle + b\,|\,1\rangle \quad \text{with} \quad |a|^2+|b|^2=1 \tag{38}$$

This means that we can write

$$a = e^{i\alpha}\cos\left(\frac{\theta}{2}\right) \quad , \quad b = e^{i\beta}\sin\left(\frac{\theta}{2}\right) \quad \text{with} \quad \alpha,\beta\in[0,2\pi]\ ,\ \theta\in[0,\pi] \tag{39}$$

Using the fact that the state is defined as a ray-vector in the Hilbert space we can factor out an overall phase and get the desired result:

$$\begin{aligned}|\,\psi\rangle &= e^{i\alpha}\cos\left(\frac{\theta}{2}\right)|\,0\rangle + e^{i\beta}\sin\left(\frac{\theta}{2}\right)|\,1\rangle = e^{i\alpha}\left(\cos\left(\frac{\theta}{2}\right)|\,0\rangle + e^{i(\beta-\alpha)}\sin\left(\frac{\theta}{2}\right)|\,1\rangle\right)\\ &\sim \cos\left(\frac{\theta}{2}\right)|\,0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|\,1\rangle \quad \text{with} \quad \phi=(\beta-\alpha)\in[0,2\pi]\end{aligned} \tag{40}$$

Since ϕ is periodic (as it can be checked from the state) and it is degenerate for $\theta = 0, \pi$, it means that these coordinates actually describe S^2.
This is how the Bloch Sphere looks like.

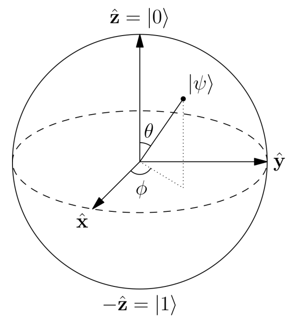

Figure 2: Representation of the Bloch Sphere.

(ii) From the condition of hermitianicity follows, since $\mathbb{1}$ and Pauli matrices are hermitian, that $\alpha, \boldsymbol{\beta}$ are real.
Furthermore:

$$1 \overset{!}{=} \operatorname{tr}\hat{\rho} = \alpha \operatorname{tr}\mathbb{1} + \boldsymbol{\beta}\cdot\operatorname{tr}\boldsymbol{\sigma} = 2\alpha \tag{41}$$

since $\operatorname{tr}\sigma_i = 0 \;\; i = 1,2,3$. It follows that $\alpha = \frac{1}{2}$.
Finally, since $(\boldsymbol{\beta}\cdot\boldsymbol{\sigma})^2 = |\boldsymbol{\beta}|^2$, it follows that the eigenvalues of $\boldsymbol{\beta}\cdot\boldsymbol{\sigma}$ are $\pm|\boldsymbol{\beta}|$. Therefore, the eigenvalues of $\hat{\rho}$ are:

$$\rho_{+,-} = \frac{1}{2} \pm |\boldsymbol{\beta}| \tag{42}$$

Since $0 \le \rho_{+,-} \le 1$, it follows that $|\boldsymbol{\beta}| \le \frac{1}{2}$.
Defining $\boldsymbol{r} = 2\boldsymbol{\beta}$, we find the announced result:

$$\hat{\rho}_{\boldsymbol{r}} = \frac{1}{2}(\mathbb{1} + \boldsymbol{r}\cdot\boldsymbol{\sigma}) \quad \text{with} \quad |\boldsymbol{r}| \le 1 \tag{43}$$

(iii) For a pure state we have $\hat{\rho}^2 = \hat{\rho}$; therefore

$$\hat{\rho}^2 = \frac{1}{4}\left[\mathbb{1} + 2\boldsymbol{r}\cdot\boldsymbol{\sigma} + (\boldsymbol{r}\cdot\boldsymbol{\sigma})^2\right] = \frac{1}{4}\left[\mathbb{1}(1+|\boldsymbol{r}|^2) + 2\boldsymbol{r}\cdot\boldsymbol{\sigma}\right] = \hat{\rho} \quad \Longleftrightarrow \quad |\boldsymbol{r}| = 1 \tag{44}$$

It follows that pure states live on the Bloch Sphere (as found in point (i)). On the other hand, it follows that mixed states live in the interior of the sphere with $|\boldsymbol{r}| < 1$.

(iv) Let's take two orthogonal states $|\,r_+\rangle, |\,r_-\rangle$; since they are pure states, to each of them is associated a vector $\boldsymbol{r}_+, \boldsymbol{r}_-$ s.t. $|\boldsymbol{r}_+| = |\boldsymbol{r}_-| = 1$.

$$\begin{aligned} \langle r_+\,|\,r_-\rangle = 0 \quad \Rightarrow \quad & |\,r_+\rangle\langle r_+\,|\,r_-\rangle\langle r_-\,| = 0 \quad \Longleftrightarrow \quad \hat{\rho}_{\boldsymbol{r}_+}\hat{\rho}_{\boldsymbol{r}_-} = 0 \quad \Longleftrightarrow \\ \Longleftrightarrow \quad & \frac{1}{4}\left[\mathbb{1} + (\boldsymbol{r}_+ + \boldsymbol{r}_-)\cdot\boldsymbol{\sigma} + (\boldsymbol{r}_+\cdot\boldsymbol{\sigma})(\boldsymbol{r}_-\cdot\boldsymbol{\sigma})\right] = 0 \end{aligned} \tag{45}$$

This implies that: $\operatorname{tr}(\hat{\rho}_{\boldsymbol{r}_+}\hat{\rho}_{\boldsymbol{r}_-}) = 0$. Using the fact that $\operatorname{tr}\sigma_i = 0$ and $\sigma_i\sigma_j = \delta_{ij}\mathbb{1} + i\epsilon_{ij}{}^k\sigma_k$ (and therefore $\operatorname{tr}(\sigma_i\sigma_j) = 2\delta_{ij}$):

$$\begin{aligned} 0 = \operatorname{tr}(\hat{\rho}_{\boldsymbol{r}_+}\hat{\rho}_{\boldsymbol{r}_-}) &= \frac{1}{4}\left[2 + 0 + \operatorname{tr}(r_+^i r_-^j \sigma_i\sigma_j)\right] = \frac{1}{4}\left[2 + r_+^i r_-^j 2\delta_{ij}\right] = \frac{1}{2}\left[1 + \boldsymbol{r}_+\cdot\boldsymbol{r}_-\right] \\ \Longleftrightarrow \quad & \boldsymbol{r}_+\cdot\boldsymbol{r}_- = -1 \end{aligned} \tag{46}$$

This means that they are anti-parallel, i.e. the corresponding states are in antipodal points in the Bloch Sphere.

(v)

$$\langle H\rangle_{\boldsymbol{r}} = \operatorname{tr}(\hat{H}\hat{\rho}_{\boldsymbol{r}}) = \frac{a}{2}\operatorname{tr}\left[\boldsymbol{B}\cdot\boldsymbol{\sigma} + (\boldsymbol{B}\cdot\boldsymbol{\sigma})(\boldsymbol{r}\cdot\boldsymbol{\sigma})\right] = \frac{a}{2}\left[0 + 2\boldsymbol{B}\cdot\boldsymbol{r}\right] = a\boldsymbol{B}\cdot\boldsymbol{r} \tag{47}$$

Just to understand better the physical correspondence with a spin 1/2 particle, notice that following the same calculation we have that for a pure state:

$$\langle \boldsymbol{r}\cdot\hat{\sigma}\rangle_{\boldsymbol{r}} = \mathrm{tr}\left((\boldsymbol{r}\cdot\hat{\sigma})\hat{\rho}_{\boldsymbol{r}}\right) = ... = \boldsymbol{r}\cdot\boldsymbol{r} = 1 \tag{48}$$

This means that $\hat{\rho}_{\boldsymbol{r}}$ describe a pure state of a particle with spin in direction $\boldsymbol{r}$.

(vi) This case corresponds to the ensemble $\{(1/2, |\,0\rangle); (1/2, |\,1\rangle)\}$. The corresponding density matrix is:

$$\hat{\rho} = \frac{1}{2}\,|\,0\rangle\,\langle 0\,| + \frac{1}{2}\,|\,1\rangle\,\langle 1\,| = \frac{1}{2}\mathbb{1} \quad \Longrightarrow \quad \boldsymbol{r} = 0 \tag{49}$$

Given the probabilities of the ensemble $\{p_k\}_{k\in\mathbb{N}}$, the entropy is given by: $S = -\sum_k p_k \log(p_k)$. In this case $p_0, p_1 = 1/2$ and therefore $S = \log(2)$.

(vii) The maximum entropy is achieved when all states have equal probability $1/\mathit{dimension}$ and this is the case of the previous point. It follows that in general the maximally entangled states lay at $\boldsymbol{r} = 0$.

(viii) As it has been shown in (i) a particle produced in direction θ, ϕ is described by the state:

$$|\,\theta,\phi\rangle = \cos\left(\frac{\theta}{2}\right)|\,0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|\,1\rangle \tag{50}$$

The density matrix describing this state is:

$$\hat{\rho}_{\theta,\phi} = |\,\theta,\phi\rangle\,\langle\theta,\phi\,| = \begin{pmatrix} \cos^2(\theta/2) & \cos(\theta/2)\sin(\theta/2)e^{-i\phi} \\ \cos(\theta/2)\sin(\theta/2)e^{i\phi} & \sin^2(\theta/2) \end{pmatrix} \tag{51}$$

Note: it corresponds to the case with $\boldsymbol{r} = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$, that is just a vector in spherical coordinate on S^2.

The probability density of being produced in one particular direction is $1/4\pi$, that is, the inverse of the surface of S^2.
The density matrix of particle produced in all directions with equal probability can be calculated as in the discrete case replacing the sum with the integral over the sphere:

$$\begin{aligned}
\hat{\rho} &= \int_{S^2} p_{\theta,\phi}\,|\,\theta,\phi\rangle\,\langle\theta,\phi\,| = \int_{S^2} \frac{1}{4\pi}\,|\,\theta,\phi\rangle\,\langle\theta,\phi\,| = \\
&= \frac{1}{4\pi}\int_0^{\pi} d\theta\,\sin(\theta)\int_0^{2\pi} d\phi \begin{pmatrix} \cos^2(\theta/2) & \cos(\theta/2)\sin(\theta/2)e^{-i\phi} \\ \cos(\theta/2)\sin(\theta/2)e^{i\phi} & \sin^2(\theta/2) \end{pmatrix} = \\
&= \frac{2\pi}{4\pi}\int_0^{\pi} d\theta\,\sin(\theta)\begin{pmatrix} \cos^2(\theta/2) & 0 \\ 0 & \sin^2(\theta/2) \end{pmatrix} = \frac{1}{2}\mathbb{1}
\end{aligned} \tag{52}$$

Therefore, as it could be expected since the amount of information is minimal, it describes a maximally entangled state.

Exercise 61 - Time dependent two level system

Consider a two level system with orthonormal basis (ONB) $|\,1\rangle$,$|\,2\rangle$. The Hamiltonian is

$$H = H_0 + V(t) \tag{53}$$

where

$$H_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}, \quad V(t) = \begin{pmatrix} 0 & \delta e^{i\omega t} \\ \delta e^{-i\omega t} & 0 \end{pmatrix} \tag{54}$$

(i) Write down an equation for the time evolution in the interaction picture. Spell it out in components. You obtain a system of two coupled differential equations.
Hint: Write $|\,\psi(t)\rangle_I$ as $|\,\psi(t)\rangle_I = c_1(t)\,|\,1\rangle + c_2(t)\,|\,2\rangle$ (two level system).

(ii) Show that one can eliminate $c_1(t)$ to obtain a differential equation for $c_2(t)$.

(iii) At $t = 0$ the system is in state $|\,1\rangle$. Show that the above equation is solved by

$$c_2(t) = Ae^{-it(\omega-\omega_{21})/2}\sin(\Omega t) \tag{55}$$

where A is a normalization constant, $\omega_{21} = (E_2 - E_1)/\hbar$ and

$$\Omega^2 = \delta^2/\hbar^2 + \frac{(\omega - \omega_{21})^2}{4} \tag{56}$$

(iv) Compute $c_1(t)$ and A.

(v) What is the probability to find the system in state $|\,2\rangle$ after the time t? Determine also the maximum (over t) probability.

(vi) Compute the previous transition probability in first order perturbation theory, taking into account again that at $t = 0$ the system is in state $|\,1\rangle$. Then compare to the exact result. In which case do the results agree?

Solution

(i) In the interaction picture holds:

$$i\hbar\partial_t\,|\,\psi(t)\rangle_I = V_I(t)\,|\,\psi(t)\rangle_I \tag{57}$$

where

$$V_I(t) = e^{\frac{i}{\hbar}H_0 t}V(t)e^{-\frac{i}{\hbar}H_0 t} \tag{58}$$

and

$$|\,\psi(t)\rangle_I = e^{\frac{i}{\hbar}H_0 t}\,|\,\psi(t)\rangle_S \tag{59}$$

Let $|\,\psi(t)\rangle_I = c_1(t)\,|\,1\rangle + c_2(t)\,|\,2\rangle = \sum_n c_n(t)\,|\,n\rangle$, as corresponds to a two level system. Therefore we can now just replace, obtaining:

$$i\hbar\partial_t\sum_n c_n(t)\,|\,n\rangle = e^{\frac{i}{\hbar}H_0 t}V(t)e^{-\frac{i}{\hbar}H_0 t}\sum_n c_n(t)\,|\,n\rangle \tag{60}$$

Acting with $\langle m\,|$ on the LHS on the previous equation, we get:

$$i\hbar\dot{c_m}(t) = e^{\frac{i}{\hbar}E_m t}\sum_n \langle m\,|\,V(t)\,|\,n\rangle\, c_n(t)e^{-\frac{i}{\hbar}E_n t} \tag{61}$$

In the basis

$$|\,1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |\,2\rangle = \begin{pmatrix}0\\1\end{pmatrix} \tag{62}$$

we straightforwardly obtain:

$$i\hbar\dot{c_1}(t) = e^{\frac{i}{\hbar}E_1 t}\delta e^{i\omega t}c_2(t)e^{-\frac{i}{\hbar}E_2 t} =: \delta e^{i(\omega-\omega_{21})t}c_2(t) \tag{63}$$

$$i\hbar\dot{c_2}(t) = e^{\frac{i}{\hbar}E_2 t}\delta e^{-i\omega t}c_1(t)e^{-\frac{i}{\hbar}E_1 t} =: \delta e^{-i(\omega-\omega_{21})t}c_1(t)\ . \tag{64}$$

(ii) Defining $\tilde{\omega} = \omega - \omega_{21}$ and differentiating with respect to the time (64), we get:

$$\dot{c_1}(t) = \frac{i\hbar}{\delta}[\ddot{c_2}(t) + i\tilde{\omega}\dot{c_2}(t)]e^{i\tilde{\omega}t} \tag{65}$$

Replacing it in (63), we finally obtain:

$$\ddot{c_2}(t) + i\tilde{\omega}\dot{c_2}(t) + \frac{\delta^2}{\hbar^2}c_2(t) = 0\ . \tag{66}$$

(iii) Use the logical ansatz $c_2(t) = Ae^{-\frac{it\tilde{\omega}}{2}}\sin\Omega t$, differentiate it twice and replace in (66), taking into account that $c_2(0) = 0$:

$$-\frac{\tilde{\omega}^2}{4}\sin\Omega t - i\tilde{\omega}\Omega\cos\Omega t - \Omega^2\sin\Omega t + \frac{\delta^2}{\hbar^2}\sin\Omega t + \frac{\tilde{\omega}^2}{2}\sin\Omega t + i\tilde{\omega}\Omega\cos\Omega t \stackrel{!}{=} 0 \Longrightarrow \Omega^2 = \frac{\delta^2}{\hbar^2} + \frac{\tilde{\omega}^2}{4} \tag{67}$$

(iv) From

$$c_1(t) = \frac{i\hbar}{\delta}\dot{c_2}(t)e^{i\tilde{\omega}t} = \frac{i\hbar}{\delta}Ae^{\frac{i\tilde{\omega}t}{2}}[\Omega\cos\Omega t - \frac{i\tilde{\omega}}{2}\sin\Omega t] \tag{68}$$

and $|c_1|^2 + |c_2|^2 = 1$ evaluated, without loss of generality and for the sake of laziness, at $t = 0$ (recall $c_2(0) = 0$), we obtain directly:

$$|c_1(0)|^2 \stackrel{!}{=} 1 \Longrightarrow A = \sqrt{\frac{\delta^2}{\delta^2 + \frac{\tilde{\omega}^2\hbar^2}{4}}} \tag{69}$$

(v) The probability to find the system in $|\,2\rangle$ is given by:

$$P(|\,2\rangle\,, t) = |c_2(t)|^2 = A^2\sin^2\Omega t \tag{70}$$

and its maximum is therefore reached whenever

$$t = t_n = \frac{1}{\Omega}\left(\frac{\pi}{2} + n\pi\right) \qquad n \in \mathbb{N} \tag{71}$$

implying:

$$P_{\max} = A^2 = \frac{\delta^2}{\delta^2 + \frac{\tilde{\omega}^2\hbar^2}{4}} \leq 1 \tag{72}$$

(vi) Plugging in $V_{21} = \delta e^{-i\omega t}$ in (c.f. equation 34 exercise 55):

$$P_{1\to 2}(t) = \frac{1}{\hbar^2}\left|\int_0^T dt_I V_{21}e^{i\omega_{21}t_I}\right|^2 \tag{73}$$

we obtain:

$$P_{1\to 2}(t) = \frac{4\delta^2}{\hbar^2(\omega_{21} - \omega)^2}\sin^2\frac{(\omega_{21} - \omega)^2 t}{2} \tag{74}$$

As a consequence, we observe that both results agree for small perturbations. Concretely, this means that δ has to be small, or more precisely

$$\delta^2 \ll (\omega - \omega_{21})^2\frac{\hbar^2}{4} \tag{75}$$

This means that $\Omega \sim |\omega - \omega_{21}|/2$ and the result agrees.

Exercise 62 - Scattering

The scattering amplitude in the first Born approximation is given by

$$f(\vartheta, \varphi) = -\frac{m}{2\pi\hbar^2}\int d^3\boldsymbol{r}e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}V(\boldsymbol{r}). \tag{76}$$

Here $\boldsymbol{k}$ is the wave vector of the incoming wave and $\boldsymbol{k}'$ is the wave vector of the outgoing wave.

(i) Consider a spherically symmetric potential $V(|\boldsymbol{r}|)$. Simplify the formula in the first Born approximation, i.e. integrate over all angles.

(ii) What is the energy of the incoming wave in terms of $\boldsymbol{k}$? Consider the low energy limit of the scattering amplitude. Show that the expression for it is to the leading order

$$f = -\frac{2m}{\hbar^2}\int_0^\infty r^2 V(r) dr. \tag{77}$$

(iii) Consider now the spherically symmetric potential well of depth V_0 and radius a, i.e. a potential

$$V(\boldsymbol{r}) = \begin{cases} -V_0 & |\boldsymbol{r}| < a \\ 0 & |\boldsymbol{r}| > a. \end{cases} \tag{78}$$

What is the scattering amplitude in this case and what is the total cross section (still in the low energy limit)?

Solution

(i) First of all, we can introduce spherical coordinates centered at the origin and such that the z-axis agrees with the direction of the vector $\boldsymbol{k}-\boldsymbol{k}'$. In that case we have

$$f(\vartheta,\varphi) = -\frac{m}{2\pi\hbar^2}\int_0^\infty r^2 dr \int_0^\pi \sin\vartheta d\vartheta \int_0^{2\pi} d\varphi V(r) e^{i|\boldsymbol{k}-\boldsymbol{k}'|r\cos\vartheta} \tag{79}$$

$$= -\frac{m}{\hbar^2}\int_0^\infty r^2 V(r) dr \int_{-1}^{+1} dy e^{i|\boldsymbol{k}-\boldsymbol{k}'|ry} \tag{80}$$

$$= -\frac{m}{\hbar^2}\int_0^\infty r^2 V(r) dr \left[\frac{e^{i|\boldsymbol{k}-\boldsymbol{k}'|ry}}{i|\boldsymbol{k}-\boldsymbol{k}'|r}\right]_{-1}^{+1} \tag{81}$$

$$= -\frac{2m}{\hbar^2|\boldsymbol{k}-\boldsymbol{k}'|}\int_0^\infty rV(r)\sin(|\boldsymbol{k}-\boldsymbol{k}'|r)dr. \tag{82}$$

(ii) The energy of the incoming wave is

$$\frac{\hbar^2|\boldsymbol{k}|^2}{2m} \tag{83}$$

so the low energy limit is the limit where $|\boldsymbol{k}| \to 0$. We can thus replace the factor

$$\frac{\sin(|\boldsymbol{k}-\boldsymbol{k}'|r)}{|\boldsymbol{k}-\boldsymbol{k}'|} \simeq r \tag{84}$$

and we immediately find the expression in the question.

(iii) Since the potential is constant, we have

$$f = \frac{2mV_0}{\hbar^2}\int_0^a r^2 dr = \frac{2ma^3V_0}{3\hbar^2}. \tag{85}$$

The total cross section is obtained by integrating the differential cross section $|f|^2$ over all spherical angles. Since f does not depend on the angles, we find

$$\sigma = \frac{16\pi m^2 a^6 V_0^2}{9\hbar^4}. \tag{86}$$

Exercise 63 - Propagator of the harmonic oscillator

In this exercise we want to calculate the propagator of the harmonic oscillator explicitly. Remember that the propagator is given by:

$$\mathcal{K}(q_F,t_F;q_I,t_I) = \lim_{N\to\infty}\int \mathrm{d}q_2...\mathrm{d}q_N \mathrm{d}p_1...\mathrm{d}p_N \prod_{j=1}^N \langle q_{j+1}\,|\,p_j\rangle\,\langle p_j\,|\,q_j\rangle\,\mathrm{e}^{-\frac{i}{\hbar}\epsilon H(p_j,q_j,t+(j-1)\epsilon)} \tag{87}$$

with the Hamiltonian of the harmonic oscillator given by:

$$H(p,q) = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}q^2 \tag{88}$$

(i) Consider the sequence of $N \times N$ matrices M_{N+1} given by

$$M_{N+1} = \begin{pmatrix} \alpha & -1 & 0 & 0 & \dots & 0 \\ -1 & \alpha & -1 & 0 & \dots & 0 \\ 0 & -1 & \alpha & -1 & \dots & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & 0 & 0 & -1 & \alpha & -1 \\ 0 & 0 & 0 & 0 & -1 & \alpha \end{pmatrix} \tag{89}$$

Show that $\det(M_{N+1}) = \alpha \det(M_N) - \det(M_{N-1})$.

(ii) Now assume that $\det(M_N) = f(\epsilon N)$ and $\alpha = 2 - \epsilon^2\omega^2$.
Show that for $\epsilon \to 0$,

$$f''(\epsilon N) = -\omega^2 f(\epsilon N) \text{ with } f(0) = 0, f'(0) = \frac{1}{\epsilon} \tag{90}$$

follows from the result of (i).

(iii) Setting $\epsilon = \frac{t_F - t_I}{N}$ show that in the limit $N \to \infty$ we have

$$\epsilon \det(M_N) \to \frac{1}{\omega}\sin(\omega(t_F - t_I)); \qquad \det(M_N) - \det(M_{N-1}) \to \cos(\omega(t_F - t_I)) \tag{91}$$

(iv) Perform the gaussian integration of p in (87) to write the propagator as

$$\mathcal{K}(q_F, t_F; q_I, t_I) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2} \int \mathrm{d}q_2 ... \mathrm{d}q_N \mathrm{e}^{\frac{im}{2\hbar\epsilon}(q_F^2 + q_I^2 - 2q_N q_F - 2q_2 q_I + \sum_{ij=2}^N (M_N)_{ij} q_i q_j - \epsilon^2\omega^2 q_I^2)} \tag{92}$$

Hint: You may use the formula for n dimensional gaussian integration given in exercise 45.

(v) Perform the Gaussian integration over q and check if the result coincides with the one obtained in Exercise 45.

Solution

(i)

$$M_{N+1} = \begin{pmatrix} \alpha & -1 & 0 & \dots & 0 \\ -1 & & & & \\ \vdots & & M_N & & \\ 0 & & & & \end{pmatrix} = \begin{pmatrix} \alpha & -1 & 0 & \dots & 0 \\ -1 & \alpha & -1 & \dots & 0 \\ \vdots & -1 & & M_{N-1} & \\ 0 & \vdots & & & \end{pmatrix}$$

Therefore the determinant is given by

$$\det(M_{N+1}) = \alpha \det(M_N) + \begin{vmatrix} -1 & -1 & 0 \\ 0 & M_{N-1} & \\ 0 & & \end{vmatrix} = \alpha \det(M_N) - \det(M_{N-1})$$

(ii) Plugging α and f into the equation for the determinant we get:

$$\begin{aligned} f(\epsilon(N+1)) &= (2 - \epsilon^2\omega^2) f(\epsilon N) - f(\epsilon(N-1)) \\ \Leftrightarrow -\omega^2 f(\epsilon N) &= \frac{f(\epsilon(N+1)) + f(\epsilon(N-1)) - 2f(\epsilon N)}{\epsilon^2} = f''(\epsilon N) \end{aligned}$$

The last step can be seen be using the definition of the derivative $f'(\epsilon N) = \frac{f(\epsilon(N+1)) - f(\epsilon N)}{\epsilon}$.
To show that the boundary conditions are fulfilled automatically we use the iterative relation for the determinant for $N = 1$:

$$\begin{aligned} \det(M_2) = \alpha = \alpha \det(M_1) - \underbrace{\det(M_0)}_{=0} \quad &\Leftrightarrow \det(M_1) = 1 \\ \Rightarrow f(0) = 0; \quad f'(0) = \frac{f(1) - f(0)}{\epsilon} &= \frac{1}{\epsilon} \end{aligned}$$

(iii) The general solution to the differential equation is given by:

$$f(\epsilon N) = A\sin(\epsilon\omega N) + B\cos(\epsilon\omega N)$$

And plugging in the boundary conditions we get $f(\epsilon N) = \frac{1}{\omega\epsilon}\sin(\omega\epsilon N)$ and therefore we get

$$\begin{aligned}
\epsilon\det(M_N) &\to \frac{1}{\omega}\sin(\omega(t_F - t_I)) \\
\det(M_N) - \det(M_{N-1}) &= \frac{\sin(\omega\epsilon N) - \sin(\omega\epsilon(N-1))}{\omega\epsilon} \to \cos(\omega(t_F - t_I))
\end{aligned}$$

(iv) The propagator is given by:

$$\begin{aligned}
\mathcal{K}(q_F, t_F; q_I, t_I) &= \frac{1}{(2\pi\hbar)^N}\int \mathrm{d}q_2 ... \mathrm{d}q_N \mathrm{d}p_1 ... \mathrm{d}p_N \prod_{j=1}^{N} \mathrm{e}^{\frac{i}{\hbar}p_j(q_{j+1}-q_j) - \frac{i}{\hbar}\epsilon\left(\frac{1}{2m}p_j^2 + \frac{m\omega^2}{2}q_j^2\right)} \\
&= \frac{1}{(2\pi\hbar)^N}\int \mathrm{d}q_2 ... \mathrm{d}q_N \mathrm{e}^{-\frac{i\epsilon m\omega^2}{2\hbar}\sum_{j=1}^N q_j^2}\int \mathrm{d}p_1 ... \mathrm{d}p_N \mathrm{e}^{\sum_{j=1}^N\left(-\frac{i\epsilon}{2\hbar m}p_j^2 + \frac{i}{\hbar}p_j(q_{j+1}-q_j)\right)} \\
&= \sqrt{\left(\frac{m}{2\pi i\hbar\epsilon}\right)^N}\int \mathrm{d}q_2 ... \mathrm{d}q_N \mathrm{e}^{\frac{im}{2\hbar\epsilon}\sum_{j=1}^N\left((q_{j+1}-q_j)^2 - \epsilon^2\omega^2 q_j^2\right)}
\end{aligned}$$

where in the last step we used the relation for integrating an N dimensional gaussian integral which was derived in problem set 7. Now we consider that the integration is done only over $\mathrm{d}q_2 ... \mathrm{d}q_N$. In the exponential however terms with $q_1 = q_I$ and $q_{N+1} = q_F$ show up. Therefore we can rewrite the exponential as:

$$\mathcal{K}(q_F, t_F; q_I, t_I) = \sqrt{\left(\frac{m}{2\pi i\hbar\epsilon}\right)^N}\int \mathrm{d}q_2 ... \mathrm{d}q_N \mathrm{e}^{\frac{im}{2\hbar\epsilon}\left(q_F^2 + q_I^2 - 2q_N q_F - 2q_2 q_I + \sum_{ij=2}^N (M_N)_{ij}q_i q_j - \epsilon^2\omega^2 q_I^2\right)}$$

(v) The exponent can be rearranged in the following way

$$\begin{aligned}
\mathcal{K}(q_F, t_F; q_I, t_I) &= \sqrt{\left(\frac{m}{2\pi i\hbar\epsilon}\right)^N}\mathrm{e}^{\frac{im}{2\hbar\epsilon}(q_F^2 + q_I^2 - \epsilon^2\omega^2 q_I^2)}\int \mathrm{d}q_2 ... \mathrm{d}q_N \mathrm{e}^{\frac{im}{2\hbar\epsilon}\left(-2q_2 q_I - 2q_N q_F + \sum_{ij=2}^N (M_N)_{ij}q_i q_j\right)} \\
&= \sqrt{\left(\frac{m}{2\pi i\hbar\epsilon}\right)^N}\mathrm{e}^{\frac{im}{2\hbar\epsilon}(q_F^2 + q_I^2 - \epsilon^2\omega^2 q_I^2)}\int \mathrm{d}q_2 ... \mathrm{d}q_N \mathrm{e}^{\frac{im}{2\hbar\epsilon}q^T M_N q - \frac{im}{\hbar\epsilon}q^T u}
\end{aligned}$$

with $u_2 = -q_I$, $u_N = -q_F$ and all the other entries $u_i = 0$. Then we can apply gaussian integration and get

$$\begin{aligned}
\mathcal{K}(q_F, t_F; q_I, t_I) &= \sqrt{\left(\frac{m}{2\pi i\hbar\epsilon}\right)^N}\sqrt{\frac{(2\pi\hbar i\epsilon)^{N-1}}{m^{N-1}\det(M_N)}}\mathrm{e}^{\frac{im}{2\hbar\epsilon}(q_F^2 + q_I^2 - \epsilon^2\omega^2 q_I^2)}\mathrm{e}^{-\frac{im}{2\hbar\epsilon}\left(q_I^2 (M_N^{-1})_{22} + q_F^2 (M_N^{-1})_{NN} + 2q_I q_F (M_N^{-1})_{2N}\right)} \\
&= \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega(t_F - t_I))}}\mathrm{e}^{\frac{im}{2\hbar\epsilon}\left((1-(M_N^{-1})_{NN})q_F^2 + (1-(M_N^{-1})_{22})q_I^2 - 2q_I q_F (M_N^{-1})_{2N} - \epsilon^2\omega^2 q_I^2\right)}
\end{aligned}$$

The inverse elements of a Matrix can be computed with the formula $(A^{-1})_{ij} = \frac{1}{\det(A)}(-1)^{i+j}\det(\tilde{A}_{ij})$ where $\tilde{A}_{ij}$ is the matrix A with the j-th row and the i-th column erased. Now we can calculate the inverse matrix elements in the exponent:

$$\begin{aligned}
(M_N^{-1})_{2N} &= \frac{1}{\det(M_N)}(-1)^N \begin{vmatrix} 1- & \alpha & ... & 0 \\ 0 & \ddots & & \vdots \\ \vdots & 0 & \ddots & \alpha \\ 0 & ... & 0 & -1 \end{vmatrix} = \frac{1}{\det(M_N)}(-1)^N(-1)^{N-2} = \frac{1}{\det(M_N)} \to \frac{\omega\epsilon}{\sin(\omega(t_F - t_I))} \\
(M^{-1})_{22} = (M^{-1})_{NN} &= \frac{\det(M_{N-1})}{\det(M_N)} \to 1 - \frac{\omega\epsilon\cos(\omega(t_F - t_I))}{\sin(\omega(t_F - t_I))}
\end{aligned}$$

Plugging this into the exponent in the propagator we get:

$$\mathcal{K}(q_F, t_F; q_I, t_I) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega(t_F - t_I))}}\exp\left\{\frac{im\omega}{2\hbar\sin(\omega(t_F - t_I))}\left((q_F^2 + q_I^2)\cos(\omega(t_F - t_I)) - 2q_F q_I\right)\right\}$$

where we omitted the term proportional to ϵ as it vanishes in the limit $\epsilon \to 0$.