3.5 Questions on the Path Integral

1. **Quantum Harmonic Oscillator:** As emphasized in lectures, the quantum harmonic oscillator provides a valuable arena in which to explore the Feynman path integral and methods of functional integration. Along with a small number of other precious examples, the path integral may be computed exactly, and the Feynman propagator explored rigorously.

   (a) Starting with the Feynman path integral, show that the propagator for the one–dimensional quantum Harmonic oscillator, $\hat{H} = \hat{p}^2/2m + m\omega^2\hat{q}^2/2$, takes the form

   $$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \left(\frac{m\omega}{2\pi i\hbar\sin\omega t}\right)^{1/2} \exp\left[\frac{i}{2\hbar}m\omega\left(\left[q_I^2 + q_F^2\right]\cot\omega t - \frac{2q_I q_F}{\sin\omega t}\right)\right].$$

   Suggest why the propagator varies periodically on the time interval t, and explain the origin of the singularities at $t = n\pi/\omega$, $n = 1, 2, \ldots$. Taking the frequency $\omega \to 0$, show that the propagator for the free particle is recovered.

   (b) Show that, the wavepacket $\psi(q, t = 0) = (2\pi a)^{-1/4}\exp[-q^2/4a]$ remains Gaussian at all subsequent times. Obtain the width $a(t)$ as a function of time.

   (c) Semiclassical limit: Taking the initial wavepacket to be of the form

   $$\psi(q, t = 0) = (2\pi a)^{-1/4}\exp\left[\frac{i}{\hbar}mvq - \frac{1}{4a}q^2\right],$$

   (which corresponds to a wavepacket centered at an initial position $q = 0$ with a velocity v) find the wavepacket at times $t > 0$, and determine the mean position, mean velocity, and mean width as a function of time.

2. **Density Matrix:** Focusing on the quantum harmonic oscillator, here we explore how real–time dynamical information can be converted into quantum statistical information.

   Using the results of the previous question, obtain the density matrix $\rho(q, q') = \langle q|e^{-\beta\hat{H}}|q'\rangle$ for the harmonic oscillator at finite temperature, $\beta = 1/T$ ($k_{\rm B} = 1$). Obtain and comment on the asymptotics: (i) $T \ll \hbar\omega$ and (ii) $T \gg \hbar\omega$. [Hint: In the high temperature case, be sure to carry out the expansion in $\hbar\omega/T$ to second order.]

3. **Winding Numbers:** In lectures, we considered the application of the Feynman path integral to model systems where trajectories could be parameterised in terms of their harmonic (Fourier) expansion. However, very often, one is interested in applications of the path integral to spaces that are not simply connected. In this case, one must include classes of trajectories which can not be simply continued. Rather, trajectories are classified by their 'winding number' on the space. To illustrate the point, let us consider the application of the path integral to a particle on a ring.

(a) Starting with the Hamiltonian $\hat{H} = -\frac{1}{2I}\frac{\partial^2}{\partial\theta^2}$, where θ denotes an angle variable, show from first principles that the quantum partition function $\mathcal{Z} = \text{tr}\ e^{-\beta\hat{H}}$ is given by

$$\mathcal{Z} = \sum_{n=-\infty}^{\infty} \exp\left[-\beta\frac{n^2}{2I}\right]. \tag{3.61}$$

(b) Formulated as a Feynman path integral, show that the quantum partition function can be cast in the form

$$\mathcal{Z} = \int_0^{2\pi} d\theta \sum_{m=-\infty}^{\infty} \int_{\substack{\theta(0)=\theta \\ \theta(\beta)=\theta(0)+2\pi m}} D\theta(\tau) \exp\left[-\frac{I}{2}\int_0^\beta d\tau \dot{\theta}^2\right].$$

(c) Varying the Eulidean action with respect to θ, show that the path integral is minimised by the classical trajectories $\bar{\theta}(\tau) = \theta + 2\pi m\tau/\beta$. Parametrising a general path as $\theta(\tau) = \bar{\theta}(\tau) + \eta(\tau)$, where $\eta(\tau)$ is a path with no net winding, show that

$$\mathcal{Z} = \mathcal{Z}_0 \sum_{m=-\infty}^{\infty} \exp\left[-\frac{I}{2}\frac{(2\pi m)^2}{\beta}\right], \tag{3.62}$$

where $\mathcal{Z}_0$ represents the quantum partition function for a free particle with open boundary conditions. Making use of the free particle propagator, show that $\mathcal{Z}_0 = \sqrt{I/2\pi\beta}$.

(d) Finally, making use of Poisson's summation formula, $\sum_m h(m) = \sum_n \int_{-\infty}^{\infty} d\phi\, h(\phi) e^{2\pi i n\phi}$, show that Eq. (3.62) coincides with Eq. (3.61).

4. †**Particle in a Periodic Potential:** In section 3.3.2 it was shown that the quantum probability amplitude for quantum mechanical tunneling can be expressed as a sum over instanton field configurations of the Euclidean action. By generalising this approach, the aim of the present problem is to explore quantum mechanical tunneling in a periodic potential. Such an analysis allows us to draw a connection to the problem of the Bloch spectrum.

(a) A quantum mechanical particle moves in a periodic lattice potential V with periodicity a. Taking the Euclidean action for the instanton connecting two neighbouring minima to be $S_{\text{inst.}}$, express the Euclidean time propagator $G(ma, na; \tau)$, with m and n integer, as a sum over instanton and anti–instanton field configurations.

(b) Making use of the identity $\delta_{qq'} = \int_0^{2\pi} e^{i(q-q')\theta} d\theta/(2\pi)$ show that

$$G(ma, na; \tau) \sim e^{\omega\tau/2} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i(n-m)\theta} \exp\left[\frac{\Delta\epsilon\tau}{\hbar} 2\cos\theta\right],$$

where our notation is taken from section 3.3.2.

(c) Keeping in mind that, in the periodic system, the eigenfunctions are Bloch states $\psi_{p\alpha}(q) = e^{ipq} u_{p\alpha}(q)$ where $u_{p\alpha}(q + ma) \equiv u_{p\alpha}(q)$ denotes the periodic part of the Bloch function, show that the propagator is compatible with a spectrum of the lowest band $\alpha = 0$, $\epsilon_p = \hbar\omega/2 - 2\Delta\epsilon \cos(pa)$.