3.6 Answers

1. (a) Making use of the Feynman path integral, the propagator can be expressed as the functional integral,

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{q(0)=q_I}^{q(t)=q_F} Dq\, e^{iS[q]/\hbar}, \qquad S[q] = \int_0^t dt\,\frac{m}{2}\left(\dot{q}^2 - \omega^2 q^2\right).$$

The evaluation of the functional integral over field configurations $q(t')$ is facilitated by parameterising the path in terms of fluctuations around the classical trajectory. Setting $q(t') = q_{\rm cl}(t') + r(t')$ where $q_{\rm cl}(t')$ satisfies the classical equation of motion $m\ddot{q}_{\rm cl} = -m\omega^2 q_{\rm cl}$, and applying the boundary conditions, one obtains the solution $q_{\rm cl}(t') = A\sin(\omega t') + B\cos(\omega t')$, with the coefficients $B = q_I$ and $A = q_F/\sin(\omega t) - q_I\cot(\omega t)$. Being Gaussian in q, the action separates as $S[q] = S[q_{\rm cl}] + S[r]$, where

$$\begin{aligned} S[q_{\rm cl}] &= \frac{m\omega^2}{2}\left[(A^2 - B^2)\frac{\sin(2\omega t)}{2\omega} + 2AB\frac{\cos(2\omega t) - 1}{2\omega}\right] \\ &= \frac{m\omega}{2}\left[(q_I^2 + q_F^2)\cot(\omega t) - \frac{2q_I q_F}{\sin(\omega t)}\right]. \end{aligned}$$

Finally, integrating over the fluctuations and applying the identity $z/\sin z = \prod_{n=1}^{\infty}(1 - z^2/\pi^2 n^2)^{-1}$ one obtains the required result, periodic in t with frequency ω, and singular at $t = n\pi/\omega$. In particular, a careful regularisation of the expression for the path integral shows that

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle \mapsto \begin{cases} \delta(q_F - q_I) & t = 2\pi n/\omega, \\ \delta(q_F + q_I) & t = \pi(2n+1)/\omega. \end{cases}$$

Physically, the origin of the singularity is clear: The harmonic oscillator is peculiar in having a spectrum with energies uniformly spaced in units of $\hbar\omega$. Noting the eigenfunction expansion $\langle q_F|e^{-i\hat{H}t\hbar}|q_I\rangle = \sum_n \langle q_F|n\rangle\langle n|q_I\rangle e^{-i\omega n t}$, this means that when $\hbar\omega \times t/\hbar = 2\pi \times$ integer there is a coherent superposition of the states and the initial state is recovered. Furthermore, since the ground state and its even integer descendents are symmetric while the odd states are antisymmetric, it is straightforward to prove the identity for the odd periods (exercise).

(b) Given the initial condition $\psi(q, t=0)$, the time evolution of the wavepacket can be determined from the propagator as $\psi(q,t) = \int_{-\infty}^{\infty} dq' \langle q|e^{-i\hat{H}t/\hbar}|q'\rangle\psi(q',0)$ from which one obtains

$$\psi(q,t) = J(t)\int_{-\infty}^{\infty} dq' \frac{1}{(2\pi a)^{1/4}} e^{-q'^2/4a} e^{\frac{i}{\hbar}\frac{m\omega}{2}\left([q^2+q'^2]\cot(\omega t) - \frac{2qq'}{\sin(\omega t)}\right)}$$

where $J(t)$ represents the time–dependent contribution arising from the fluctuations around the classical trajectory. Being Gaussian in q', the integral can be performed explicitly. Setting $\alpha = 1/2a - im\omega\cot(\omega t)/\hbar$, $\beta = im\omega q/(\hbar\sin(\omega t))$, and performing the Gaussian integral over q', one obtains

$$\psi(q,t) = J(t)\frac{1}{(2\pi a)^{1/4}}\sqrt{\frac{2\pi}{\alpha}} e^{\beta^2/2\alpha}\exp\left[\frac{i}{2\hbar} m\omega q^2\cot(\omega t)\right]$$

where $\beta^2/2\alpha = -(1+i\kappa\cot(\omega t))q^2/4a(t)$. Rearranging terms, it is straightforward to show that $\psi(q,t) = (2\pi a(t))^{-1/4}\exp[-\frac{q^2}{4a(t)}]e^{i\varphi(q,t)}$, where $a(t) = a[\cos^2(\omega t) + \kappa^{-2}\sin^2(\omega t)]$, $\kappa = 2am\omega/\hbar$ and $\varphi(q,t)$ represents a pure phase.[42] As required, under the action of the propagator, the normalisation of the wavepacket is preserved. (A graphical representation of the time evolution is shown in Fig. 3.13a.) Note that, if $a = \hbar/2m\omega$ (i.e. $\kappa = 1$), $a(t) = a$ for all times — i.e. it is a pure eigenstate.

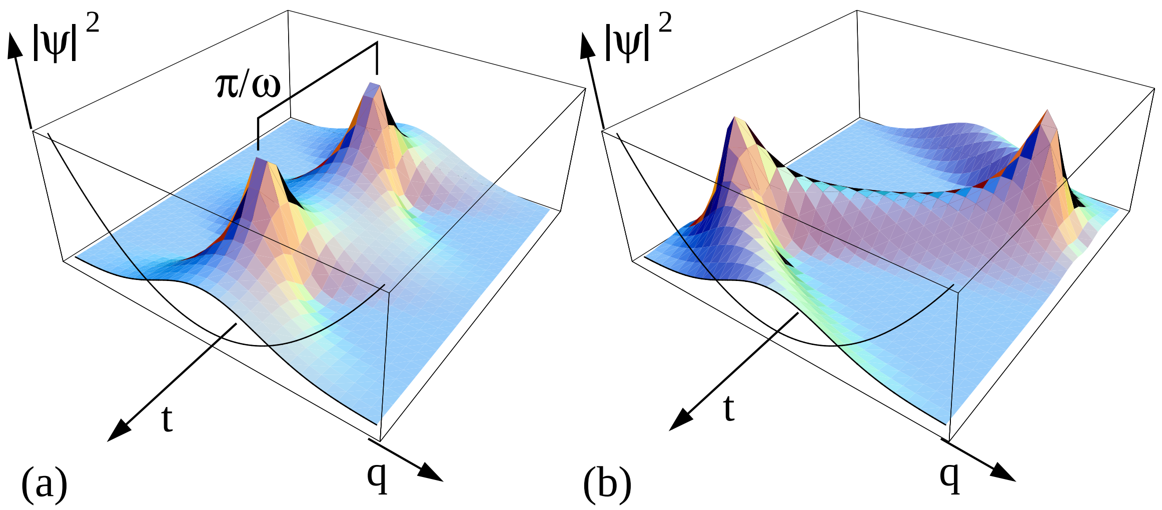

Figure 3.13: (a) Variation of a "stationary" Gaussian wavepacket in the harmonic oscillator taken from the solution, and (b) variation of the moving wavepacket.

(c) Still of a Gaussian form, the integration can again be performed explicitly for the new initial condition. In this case, we obtain an expression of the form above but with $\beta = \frac{i}{\hbar}\frac{m\omega}{\sin(\omega t)}(q - \frac{v}{\omega}\sin(\omega t))$. Reading off the coefficients, we find that the position and velocity of the wavepacket have the form $q_0(t) = (v/\omega)\sin(\omega t)$, $v(t) = v\cos(\omega t)$ coinciding with that of the classical dynamics. Note that, as above, the width $a(t)$ of the wavepacket oscillates at frequency ω. (A graphical representation of the time evolution is shown in Fig. 3.13b.)

2. The density matrix can be deduced from the general solution of the previous question. Turning to the Euclidean time formulation,

$$\begin{aligned}\rho(q,q') &= \langle q|e^{-\beta H}|q'\rangle = \langle q|e^{-(i/\hbar)H(\hbar\beta/i)}|q'\rangle \\ &= \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right)^{1/2}\exp\left[-\frac{m\omega}{2\hbar}\left((q^2+q'^2)\coth(\beta\hbar\omega) - \frac{2qq'}{\sinh(\beta\hbar\omega)}\right)\right].\end{aligned}$$

(i) In the low temperature limit $T \ll \hbar\omega$ ($\beta\hbar\omega \gg 1$), $\coth(\beta\hbar\omega) \to 1$, $\sinh(\beta\hbar\omega) \to e^{\beta\hbar\omega}/2$, and

$$\rho(q,q') \simeq \left(\frac{m\omega}{\pi\hbar e^{\beta\hbar\omega}}\right)^{1/2}\exp\left[-\frac{m\omega}{2\hbar}(q^2+q'^2)\right] = \langle q|n=0\rangle\, e^{-\beta E_0}\,\langle n=0|q'\rangle\,.$$

[42] For completeness, we note that $\varphi(q,t) = -\frac{1}{2}\tan^{-1}(\frac{1}{\kappa}\cot(\omega t)) - \frac{\kappa q^2}{4a}\cot(\omega t)(\frac{a}{a(t)} - 1)$.

(ii) Using the relation $\coth(x) \overset{x\ll 1}{=} 1/x - x/3 + \ldots$ and $1/\sinh(x) \overset{x\ll 1}{=} 1/x - x/6 + \ldots$, the high temperature expansion ($T \gg \hbar\omega$) of the density operator obtains

$$\rho(q,q') \simeq \left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2} e^{-m(q-q')^2/2\beta\hbar^2} \exp\left[-\frac{\hbar\beta m\omega^2}{6\hbar}(q^2 + q'^2 + qq')\right] \simeq \delta(q-q') e^{-\frac{\beta m\omega^2 q^2}{2}},$$

i.e. one recovers the classical Maxwell–Boltzmann distribution!

3. (a) Solving the Schrödinger equation, the wavefunctions obeying periodic boundary conditions take the form $\psi_n = e^{in\theta}/\sqrt{2\pi}$, n integer, and the eigenvalues are given by $E_n = n^2/2I$. Cast in the eigenbasis representation, the partition function assumes the form (3.61).

(b) Interpreted as a Feynman path integral, the quantum partition function takes the form of a propagator with

$$\mathcal{Z} = \int_0^{2\pi} d\theta \, \langle\theta|e^{-\beta\hat{H}}|\theta\rangle = \int_0^{2\pi} d\theta \int_{\theta(\beta)=\theta(0)=\theta} D\theta(\tau) \exp\left[-\int_0^\beta d\tau \frac{I}{2}\dot{\theta}^2\right].$$

The trace implies that paths $\theta(\tau)$ must start and finish at the same point. However, to accommodate the invariance of the field configuration θ under translation by 2π we must must impose the boundary conditions shown in the question.

(c) Varying the action with respect to θ we obtain the classical equation $I\ddot{\theta} = 0$. Solving this equation subject to the boundary conditions, we obtain the solution given in the question. Evaluating the Euclidean action, one finds

$$\int_0^\beta (\partial_\tau\theta)^2 d\tau = \int_0^\beta \left[\frac{2\pi m}{\beta} + \partial_\tau\eta\right]^2 d\tau = \beta\left(\frac{2\pi m}{\beta}\right)^2 + \int_0^\beta (\partial_\tau\eta)^2 d\tau.$$

Thus, one obtains the partition function (3.62), where

$$\mathcal{Z}_0 = \int D\eta(\tau) \exp\left[-\frac{I}{2}\int_0^\beta (\partial_\tau\eta)^2 d\tau\right] = \sqrt{\frac{2\pi I}{\beta}}.$$

denotes the free particle partition function. The latter can be obtained from direct evaluation of the free particle propagator.

(d) Applying the Poisson summation formula with $h(x) = \exp[-\frac{(2\pi)^2 I}{2\beta}x^2]$, one finds that

$$\sum_{m=-\infty}^{\infty} e^{-\frac{(2\pi)^2 I m^2}{2\beta}} = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} d\phi \, e^{-\frac{(2\pi)^2 I}{2\beta}\phi^2 + 2\pi i n\phi} = \sqrt{\frac{\beta}{2\pi I}} \sum_{n=-\infty}^{\infty} e^{-\frac{\beta}{2I}n^2}.$$

Multiplication with $\mathcal{Z}_0$ obtains the result.

4. (a) In the double well potential, the extremal field configurations of the Euclidean action involve consecutive sequences of instanton/anti–instanton pairs. However, in the periodic potential, the q instantons and q' anti–instantons can appear in any sequence provided only that $q - q' = n - m$. In this case, the Feynman amplitude takes the form

$$G(ma, na; \tau) \sim \sum_{q=0}^{\infty} \sum_{q'=0}^{\infty} \frac{\delta_{q-q',n-m}}{q!\,q'!} (\tau K e^{-S_{\text{inst.}}/\hbar})^{q+q'}$$

(b) To evaluate the instanton summation, one may make use of the identity $\delta_{q-q',n-m} = \int_0^{2\pi} e^{i(q-q'-n+m)\theta} d\theta/(2\pi)$. As a result, one obtains

$$\begin{aligned} G(ma, na; \tau) &\sim e^{\omega\tau/2} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i(n-m)\theta} \sum_{q=0}^{\infty} \frac{(\tau K e^{i\theta} e^{-S_{\text{inst.}}/\hbar})^q}{q!} \sum_{q'=0}^{\infty} \frac{(\tau K e^{-i\theta} e^{-S_{\text{inst.}}/\hbar})^{q'}}{q'!} \\ &\sim e^{\omega\tau/2} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i(n-m)\theta} \exp\left[\frac{\Delta\epsilon\tau}{\hbar} e^{i\theta}\right] \exp\left[\frac{\Delta\epsilon\tau}{\hbar} e^{-i\theta}\right] \end{aligned}$$

from which one obtains the required result.

(c) Expanded in terms of the Bloch states of the lowest band of the periodic potential $\alpha = 0$, one obtains

$$G(ma, na; \tau) = \sum_p \psi_p^*(ma)\psi_p(na) e^{-i\epsilon_p\tau/\hbar} = \sum_p |u_p(0)|^2 e^{ip(n-m)a} e^{-i\epsilon_p\tau/\hbar}$$

Interpreting $\theta = pa$, and taking $|u_p(0)|^2 = \text{const.}$ independent of p, one can draw the correspondence $\epsilon_p = \hbar\omega/2 - 2\Delta\epsilon\cos(pa)$.