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Problem Set 1: Solution

1. **Heisenberg's uncertainty principle** (3+2 points)

(a) The squared standard deviation of an operator $\hat{A}$ in a normalized quantum state $|\psi\rangle$ is defined by $\langle(\Delta\hat{A})^2\rangle$, where $\langle\cdots\rangle$ stands for the expectation value in $|\psi\rangle$ and $\Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle$. For the position operator $\hat{x}$ and momentum operator $\hat{p}$, prove Heisenberg's uncertainty principle

$$\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{p}^2)\rangle \geq \frac{\hbar^2}{4}\,.$$

(b) The eigenstates of the harmonic oscillator Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$ satisfy $\hat{H}|n\rangle = (n+\frac{1}{2})\hbar\omega|n\rangle$. Calculate $\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{p}^2)\rangle$ for each eigenstate $|n\rangle$ and verify that Heisenberg's uncertainty principle is not violated.

Solution: (a) The proof of Heisenberg's uncertainty principle goes as follows:

$$\begin{aligned}
\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{p}^2)\rangle &= \langle\psi|\Delta\hat{x}\Delta\hat{x}|\psi\rangle\langle\psi|\Delta\hat{p}\Delta\hat{p}|\psi\rangle \qquad \Leftarrow \text{define } |\psi_1\rangle = \Delta\hat{x}|\psi\rangle \text{ and } |\psi_2\rangle = \Delta\hat{p}|\psi\rangle \\
&= \langle\psi_1|\psi_1\rangle\langle\psi_2|\psi_2\rangle \qquad \Leftarrow \text{use Cauchy-Schwarz inequality} \\
&\geq |\langle\psi_1|\psi_2\rangle|^2 \\
&= |\langle\psi|\Delta\hat{x}\Delta\hat{p}|\psi\rangle|^2 \qquad \Leftarrow \text{use } \Delta\hat{x}\Delta\hat{p} = \frac{1}{2}[\Delta\hat{x},\Delta\hat{p}] + \frac{1}{2}\{\Delta\hat{x},\Delta\hat{p}\} = \frac{i\hbar}{2} + \frac{1}{2}\{\Delta\hat{x},\Delta\hat{p}\} \\
&= \left|\langle\psi|(\frac{i\hbar}{2} + \frac{1}{2}\{\Delta\hat{x},\Delta\hat{p}\})|\psi\rangle\right|^2 \qquad \Leftarrow |\psi\rangle \text{ is normalized} \\
&= \left|\frac{i\hbar}{2} + \frac{1}{2}\langle\psi|\{\Delta\hat{x},\Delta\hat{p}\}|\psi\rangle\right|^2 \qquad \Leftarrow \{\Delta\hat{x},\Delta\hat{p}\} \text{ is Hermitian, so } \langle\psi|\{\Delta\hat{x},\Delta\hat{p}\}|\psi\rangle \text{ is real.} \\
&= \frac{\hbar^2}{4} + \frac{1}{4}|\langle\psi|\{\Delta\hat{x},\Delta\hat{p}\}|\psi\rangle|^2 \\
&\geq \frac{\hbar^2}{4}.
\end{aligned}$$

(b) The bosonic representation of $\hat{x}$ and $\hat{p}$ which diagonalizes the harmonic oscillator Hamiltonian is given by $\hat{x} = \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}(\hat{a}+\hat{a}^\dagger)$ and $\hat{p} = -\frac{i}{\sqrt{2}}\sqrt{m\omega\hbar}(\hat{a}-\hat{a}^\dagger)$, where $\hat{a}^\dagger|n\rangle = (n+1)|n\rangle$ and $\hat{a}|n\rangle = n|n-1\rangle$ $(n = 0, 1, \ldots)$. By using the bosonic representation, we obtain

$$\begin{aligned}
\langle n|\hat{x}|n\rangle &= \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}\langle n|(\hat{a}+\hat{a}^\dagger)|n\rangle = 0, \\
\langle n|\hat{p}|n\rangle &= -\frac{i}{\sqrt{2}}\sqrt{m\omega\hbar}\langle n|(\hat{a}-\hat{a}^\dagger)|n\rangle = 0.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\langle n|(\Delta\hat{x})^2|n\rangle &= \langle n|\hat{x}^2|n\rangle - (\langle n|\hat{x}|n\rangle)^2 \\
&= \frac{\hbar}{2m\omega}\langle n|(\hat{a}+\hat{a}^\dagger)^2|n\rangle - 0 \\
&= \frac{\hbar}{2m\omega}\langle n|(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|n\rangle \qquad \Leftarrow \text{use } \hat{a}\hat{a}^\dagger = [\hat{a},\hat{a}^\dagger] + \hat{a}^\dagger\hat{a} = 1 + \hat{a}^\dagger\hat{a} \\
&= \frac{\hbar}{2m\omega}\langle n|(1 + 2\hat{a}^\dagger\hat{a})|n\rangle \\
&= \frac{\hbar}{2m\omega}(2n+1),
\end{aligned}$$

and

$$\begin{aligned}
\langle n|(\Delta\hat{p})^2|n\rangle &= \langle n|\hat{p}^2|n\rangle - (\langle n|\hat{p}|n\rangle)^2 \\
&= -\frac{m\omega\hbar}{2}\langle n|(\hat{a}-\hat{a}^\dagger)^2|n\rangle - 0 \\
&= -\frac{m\omega\hbar}{2}\langle n|(-\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a})|n\rangle \\
&= \frac{m\omega\hbar}{2}\langle n|(1+2\hat{a}^\dagger\hat{a})|n\rangle \\
&= \frac{m\omega\hbar}{2}(2n+1).
\end{aligned}$$

Thus, we have $\langle n|(\Delta\hat{x})^2|n\rangle\langle n|(\Delta\hat{p})^2|n\rangle = (2n+1)^2\frac{\hbar^2}{4} \geq \frac{\hbar^2}{4}$, so the Heisenberg's uncertainty relation is not violated. In fact, the bound is saturated in the ground state $|0\rangle$, which is a Gaussian wave packet in both coordinate and momentum spaces.

2. **Path integral for a free particle** (5 points)

For a free particle in one dimension, the Hamiltonian is given by $\hat{H} = \frac{\hat{p}^2}{2m}$. Calculate the propagator

$$G(x', t'; x, t) = \langle x'|e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|x\rangle$$

by using the path integral approach.

Solution: We devide the evolution time into N time-slices, $N\Delta t = t' - t$. Then, the propagator is given by

$$\begin{aligned}
&G(x', t'; x, t) \\
=\ &\langle x'|e^{-\frac{i}{\hbar}\hat{H}\Delta t}\cdots e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x\rangle \qquad \Leftarrow \text{insert complete basis in coordinate space} \\
=\ &\int \prod_{k=1}^{N-1} dx_k\ \langle x'|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_{N-1}\rangle\langle x_{N-1}|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_{N-2}\rangle\cdots\langle x_2|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_1\rangle\langle x_1|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x\rangle, \qquad (1)
\end{aligned}$$

where the propagator for a small time interval is given by

$$\begin{aligned}
&\langle x_{k+1}|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_k\rangle \\
=\ &\int_{-\infty}^{\infty} dp_k\ \langle x_{k+1}|p_k\rangle\langle p_k|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_k\rangle \qquad \Leftarrow \text{complete basis in momentum space inserted} \\
\simeq\ &\int_{-\infty}^{\infty} dp_k\ \langle x_{k+1}|p_k\rangle\langle p_k|(1-\frac{i}{\hbar}\hat{H}\Delta t)|x_k\rangle \qquad \Leftarrow \text{use } \langle p_k|\hat{H}|x_k\rangle = \frac{p_k^2}{2m}\langle p_k|x_k\rangle \\
=\ &\int_{-\infty}^{\infty} dp_k\ \left(1-\frac{i}{\hbar}\frac{p_k^2}{2m}\Delta t\right)\langle x_{k+1}|p_k\rangle\langle p_k|x_k\rangle \qquad \Leftarrow \text{use } \langle p_k|x_k\rangle = \frac{e^{-\frac{i}{\hbar}p_k x_k}}{\sqrt{2\pi\hbar}},\ \langle x_{k+1}|p_k\rangle = \frac{e^{\frac{i}{\hbar}p_k x_{k+1}}}{\sqrt{2\pi\hbar}} \\
\simeq\ &\int_{-\infty}^{\infty} \frac{dp_k}{2\pi\hbar}\ e^{-\frac{i}{\hbar}\frac{p_k^2}{2m}\Delta t + \frac{i}{\hbar}p_k(x_{k+1}-x_k)} \qquad \Leftarrow \text{complete square} \\
=\ &\int_{-\infty}^{\infty} \frac{dp_k}{2\pi\hbar}\ e^{-\frac{i\Delta t}{2m\hbar}[p_k - \frac{m}{\Delta t}(x_{k+1}-x_k)]^2 + \frac{im}{2\hbar\Delta t}(x_{k+1}-x_k)^2} \qquad \Leftarrow \text{Gaussian integral } \int_{-\infty}^{\infty} dp\ e^{-a(p+b)^2} = \sqrt{\frac{\pi}{a}} \\
=\ &\frac{1}{2\pi\hbar}\sqrt{\frac{\pi}{\frac{i}{\hbar}\frac{1}{2m}\Delta t}}e^{\frac{im}{2\hbar\Delta t}(x_{k+1}-x_k)^2} \\
=\ &\sqrt{\frac{m}{2\pi i\hbar\Delta t}}e^{\frac{im}{2\hbar\Delta t}(x_{k+1}-x_k)^2}. \qquad (2)
\end{aligned}$$

Then, substituting (1) into (2) leads to

$$G(x', t'; x, t) = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2}\int\prod_{k=1}^{N-1} dx_k\ \exp\left[\sum_{k=0}^{N-1}\frac{im}{2\hbar\Delta t}(x_{k+1}-x_k)^2\right], \qquad (3)$$

where we have defined $x_0 = x$ and $x_N = x'$ for simplying the expression. At this step, there are several ways to proceed with (3). Below two approaches are provided.

Approach 1: We could *successively* perform Gaussian integrations ($x_1 \to x_2 \to \cdots \to x_{N-1}$). For instance, the integration over x_1 is given by

$$\begin{aligned}
&\int_{-\infty}^{\infty} dx_1 \ \exp\left[\frac{im}{2\hbar\Delta t}(x_2-x_1)^2 + \frac{im}{2\hbar\Delta t}(x_1-x_0)^2\right] \\
=& \int_{-\infty}^{\infty} dx_1 \ \exp\left\{\frac{im}{2\hbar\Delta t}[2x_1^2 - 2(x_2+x_0)x_1 + (x_2^2+x_0^2)]\right\} \quad \Leftarrow \text{complete square} \\
=& \int_{-\infty}^{\infty} dx_1 \ \exp\left\{\frac{im}{2\hbar\Delta t}\left[2\left(x_1 - \frac{x_2+x_0}{2}\right)^2 - \frac{1}{2}(x_2+x_0)^2 + (x_2^2+x_0^2)\right]\right\} \\
=& \int_{-\infty}^{\infty} dx_1 \ \exp\left\{\frac{im}{2\hbar\Delta t}\left[2\left(x_1 - \frac{x_2+x_0}{2}\right)^2 + \frac{1}{2}(x_2-x_0)^2\right]\right\} \\
=& \int_{-\infty}^{\infty} dx_1 \ \exp\left[\frac{im}{\hbar\Delta t}\left(x_1 - \frac{x_2+x_0}{2}\right)^2\right] \exp\left[\frac{im}{4\hbar\Delta t}(x_2-x_0)^2\right] \quad \Leftarrow \text{Gaussian integral} \\
=& \sqrt{\frac{\pi\hbar\Delta t}{-im}} \exp\left[\frac{im}{4\hbar\Delta t}(x_2-x_0)^2\right]. \qquad (4)
\end{aligned}$$

As a side remark, we note that, after taking into account a prefactor, the calculation in (4) is just the propagator for the time-slice $2\Delta t$

$$\begin{aligned}
G(x_2, 2\Delta t; x_0, 0) &= \langle x_2|e^{-\frac{i}{\hbar}\hat{H}(2\Delta t)}|x_0\rangle \\
&= \langle x_2|e^{-\frac{i}{\hbar}\hat{H}\Delta t}e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_0\rangle \\
&= \int dx_1 \ \langle x_2|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_1\rangle\langle x_1|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|x_0\rangle \quad \Leftarrow \text{use Eq. (2)} \\
&= \frac{m}{2\pi i\hbar\Delta t}\int_{-\infty}^{\infty} dx_1 \ \exp\left[\frac{im}{2\hbar\Delta t}(x_2-x_1)^2 + \frac{im}{2\hbar\Delta t}(x_1-x_0)^2\right] \quad \Leftarrow \text{use Eq. (4)} \\
&= \frac{m}{2\pi i\hbar\Delta t}\sqrt{\frac{\pi\hbar\Delta t}{-im}} \exp\left[\frac{im}{4\hbar\Delta t}(x_2-x_0)^2\right] \\
&= \sqrt{\frac{m}{4\pi i\hbar\Delta t}} \exp\left[\frac{im}{4\hbar\Delta t}(x_2-x_0)^2\right].
\end{aligned}$$

Now we continue with (3). After substituting (4) into (3), we perform the Gaussian integration over x_2

$$\begin{aligned}
&\int_{-\infty}^{\infty} dx_2 \ \exp\left[\frac{im}{2\hbar\Delta t}(x_3-x_2)^2 + \frac{im}{4\hbar\Delta t}(x_2-x_0)^2\right] \\
=& \int_{-\infty}^{\infty} dx_2 \ \exp\left\{\frac{im}{4\hbar\Delta t}[2(x_3-x_2)^2 + (x_2-x_0)^2]\right\} \\
=& \int_{-\infty}^{\infty} dx_2 \ \exp\left\{\frac{im}{4\hbar\Delta t}[3x_2^2 - 2(2x_3+x_0)x_2 + (2x_3^2+x_0^2)]\right\} \quad \Leftarrow \text{complete square} \\
=& \int_{-\infty}^{\infty} dx_2 \exp\left\{\frac{im}{4\hbar\Delta t}\left[3\left(x_2 - \frac{2x_3+x_0}{3}\right)^2 - \frac{1}{3}(2x_3+x_0)^2 + (2x_3^2+x_0^2)\right]\right\} \\
=& \int_{-\infty}^{\infty} dx_2 \ \exp\left\{\frac{im}{4\hbar\Delta t}\left[3\left(x_2 - \frac{2x_3+x_0}{3}\right)^2 + \frac{2}{3}(x_3-x_0)^2\right]\right\} \\
=& \int_{-\infty}^{\infty} dx_1 \ \exp\left[\frac{3im}{4\hbar\Delta t}\left(x_2 - \frac{2x_3+x_0}{3}\right)^2\right] \exp\left[\frac{im}{6\hbar\Delta t}(x_3-x_0)^2\right] \quad \Leftarrow \text{Gaussian integral} \\
=& \sqrt{\frac{4\pi\hbar\Delta t}{-3im}} \exp\left[\frac{im}{6\hbar\Delta t}(x_3-x_0)^2\right]. \qquad (5)
\end{aligned}$$

Thus, we could proceed with the Gaussian integration in (3), and the integration over x_k ($k = 1, \ldots, N-1$)

is given by

$$
\begin{aligned}
& \int_{-\infty}^{\infty} dx_k \ \exp\left[\frac{im}{2\hbar\Delta t}(x_{k+1}-x_k)^2 + \frac{im}{2k\hbar\Delta t}(x_k - x_0)^2\right] \\
= & \int_{-\infty}^{\infty} dx_k \ \exp\left\{\frac{im}{2\hbar\Delta t}\left[(x_{k+1}-x_k)^2 + \frac{1}{k}(x_k-x_0)^2\right]\right\} \\
= & \int_{-\infty}^{\infty} dx_k \ \exp\left\{\frac{im}{2\hbar\Delta t}\left[\frac{k+1}{k}x_k^2 - 2\left(x_{k+1}+\frac{1}{k}x_0\right)x_k + \left(x_{k+1}^2+\frac{1}{k}x_0^2\right)\right]\right\} \quad \Leftarrow \text{complete square} \\
= & \int_{-\infty}^{\infty} dx_k \ \exp\left\{\frac{im}{2\hbar\Delta t}\left[\frac{k+1}{k}\left(x_k - \frac{kx_{k+1}+x_0}{k+1}\right)^2 - \frac{k+1}{k}\left(\frac{kx_{k+1}+x_0}{k+1}\right)^2 + \left(x_{k+1}^2+\frac{1}{k}x_0^2\right)\right]\right\} \\
= & \int_{-\infty}^{\infty} dx_k \ \exp\left\{\frac{im}{2\hbar\Delta t}\left[\frac{k+1}{k}\left(x_k - \frac{kx_{k+1}+x_0}{k+1}\right)^2 + \frac{(x_{k+1}-x_0)^2}{k+1}\right]\right\} \\
= & \int_{-\infty}^{\infty} dx_k \ \exp\left[\frac{(k+1)im}{2k\hbar\Delta t}\left(x_2 - \frac{2x_3+x_0}{3}\right)^2\right] \exp\left[\frac{im(x_{k+1}-x_0)^2}{2(k+1)\hbar\Delta t}\right] \quad \Leftarrow \text{Gaussian integral} \\
= & \sqrt{\frac{k}{k+1}\frac{2\pi\hbar\Delta t}{-im}} \exp\left[\frac{im(x_{k+1}-x_0)^2}{2(k+1)\hbar\Delta t}\right]. \qquad (6)
\end{aligned}
$$

This leads to an explicit expression for the propagator in (3)

$$
\begin{aligned}
& G(x',t';x,t) \\
= & \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2}\left(\prod_{k=1}^{N-1}\sqrt{\frac{k}{k+1}\frac{2\pi\hbar\Delta t}{-im}}\right) \exp\left[\frac{im(x_N-x_0)^2}{2N\hbar\Delta t}\right] \quad \Leftarrow \text{use } x_0 = x,\ x_N = x' \\
= & \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2}\left(\frac{2\pi\hbar\Delta t}{-im}\right)^{(N-1)/2}\sqrt{\frac{N-1}{N}\frac{N-2}{N-1}\cdots\frac{1}{2}} \exp\left[\frac{im(x'-x)^2}{2N\hbar\Delta t}\right] \\
= & \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2}\sqrt{\frac{1}{N}} \exp\left[\frac{im(x'-x)^2}{2N\hbar\Delta t}\right] \\
= & \sqrt{\frac{m}{2\pi i\hbar N\Delta t}} \exp\left[\frac{im(x'-x)^2}{2N\hbar\Delta t}\right] \quad \Leftarrow \text{use } N\Delta t = t'-t \\
= & \sqrt{\frac{m}{2\pi i\hbar(t'-t)}} \exp\left[\frac{im(x'-x)^2}{2\hbar(t'-t)}\right]. \qquad (7)
\end{aligned}
$$

Approach 2: The multidimensional Gaussian integration in (3) could also be performed by using the following formula:

$$
\begin{aligned}
\int \prod_{n=1}^{N} dx_n \ e^{-\frac{1}{2}x^TAx - x^Ty} &= \int \prod_{n=1}^{N} dx_n \ e^{-\frac{1}{2}(x^T-y^TA^{-1})A(x-A^{-1}y^T)y+\frac{1}{2}y^TA^{-1}y} \\
&= (2\pi)^{N/2}(\det A)^{-1/2}e^{\frac{1}{2}y^TA^{-1}y}, \qquad (8)
\end{aligned}
$$

where x and y are column vectors, $x = (x_1, x_2, \ldots, x_N)^T$ and $y = (y_1, y_2, \ldots, y_N)^T$, and A is a $N \times N$ symmetric matrix. You may prove (8) by diagonalizing A.

Let us rewrite the integral in (3) as

$$
\begin{aligned}
& \int \prod_{k=1}^{N-1} dx_k \ \exp\left[\sum_{k=0}^{N-1}\frac{im}{2\hbar\Delta t}(x_{k+1}-x_k)^2\right] \\
= & \int \prod_{k=1}^{N-1} dx_k \ \exp\left[\frac{im}{\hbar\Delta t}(x_1^2+\cdots+x_{N-1}^2 - x_0x_1 - x_1x_2 - \cdots - x_{N-1}x_N) + \frac{im}{2\hbar\Delta t}(x_0^2+x_N^2)\right] \\
= & \int \prod_{k=1}^{N-1} dx_k \ \exp\left[-\frac{1}{2}x^TAx - x^Ty + \frac{im}{2\hbar\Delta t}(x_0^2+x_N^2)\right] \quad \Leftarrow \text{use Eq. (8)} \\
= & (2\pi)^{(N-1)/2}(\det A)^{-1/2}e^{\frac{1}{2}y^TA^{-1}y} \exp\left[\frac{im}{2\hbar\Delta t}(x_0^2+x_N^2)\right], \qquad (9)
\end{aligned}
$$

where $x=(x_1,x_2,\ldots,x_{N-1})^T$, $y=\frac{im}{\hbar\Delta t}(x_0,0,\ldots,0,x_N)^T$, and A is given by

$$A=-\frac{2im}{\hbar\Delta t}\begin{pmatrix} 1 & -1/2 & & & & \\ -1/2 & 1 & -1/2 & & & \\ & -1/2 & 1 & -1/2 & & \\ & & -1/2 & 1 & & \\ & & & & \ddots & -1/2 \\ & & & & -1/2 & 1 \end{pmatrix}_{(N-1)\times(N-1)}. \tag{10}$$

According to (8), we need to calculate $\det A$ and four matrix entries of A^{-1}. We observe that the matrix A, up to an irrelevant overall factor, is the same as the single-particle Hamiltonian for a 1D tight-binding model with *open* boundary condition, whose eigenvectors take the form of discretized standing waves. More explicitly, the eigenvalue equation for A is given by

$$Aw_q=\lambda_q w_q, \tag{11}$$

where $q=1,\ldots,N-1$ and $w_q=\sqrt{\frac{2}{N}}(\sin\frac{\pi q}{N},\sin\frac{2\pi q}{N},\sin\frac{3\pi q}{N},\sin\frac{4\pi q}{N},\ldots,\sin\frac{(N-1)\pi q}{N})^T$. It is straightforward to show that w_q are orthonormal and complete, $w_q^T w_{q'}=\delta_{qq'}\ \forall q,q'$. Let us verify that they are indeed eigenvectors of A and determine the corresponding eigenvalues λ_q,

$$\begin{aligned}
Aw_q &= -\frac{2im}{\hbar\Delta t}\sqrt{\frac{2}{N}}\begin{pmatrix} 1 & -1/2 & & & & \\ -1/2 & 1 & -1/2 & & & \\ & -1/2 & 1 & -1/2 & & \\ & & -1/2 & 1 & & \\ & & & & \ddots & -1/2 \\ & & & & -1/2 & 1 \end{pmatrix}\begin{pmatrix}\sin\frac{\pi q}{N}\\ \sin\frac{2\pi q}{N}\\ \sin\frac{3\pi q}{N}\\ \sin\frac{4\pi q}{N}\\ \vdots \\ \sin\frac{(N-1)\pi q}{N}\end{pmatrix}\\
&= -\frac{2im}{\hbar\Delta t}\sqrt{\frac{2}{N}}\begin{pmatrix}\sin\frac{\pi q}{N}-\frac{1}{2}\sin\frac{2\pi q}{N}\\ \sin\frac{2\pi q}{N}-\frac{1}{2}(\sin\frac{\pi q}{N}+\sin\frac{3\pi q}{N})\\ \sin\frac{3\pi q}{N}-\frac{1}{2}(\sin\frac{2\pi q}{N}+\sin\frac{4\pi q}{N})\\ \sin\frac{4\pi q}{N}-\frac{1}{2}(\sin\frac{3\pi q}{N}+\sin\frac{5\pi q}{N})\\ \vdots \\ \sin\frac{(N-1)\pi q}{N}-\frac{1}{2}(\sin\frac{(N-2)\pi q}{N}+\sin\frac{N\pi q}{N})\end{pmatrix} \qquad \Leftarrow \text{use } \sin\frac{N\pi q}{N}=\sin(\pi q)=0\\
&= -\frac{2im}{\hbar\Delta t}\sqrt{\frac{2}{N}}\begin{pmatrix}\sin\frac{\pi q}{N}-\sin\frac{\pi q}{N}\cos\frac{\pi q}{N}\\ \sin\frac{2\pi q}{N}-\sin\frac{2\pi q}{N}\cos\frac{\pi q}{N}\\ \sin\frac{3\pi q}{N}-\sin\frac{3\pi q}{N}\cos\frac{\pi q}{N}\\ \sin\frac{4\pi q}{N}-\sin\frac{4\pi q}{N}\cos\frac{\pi q}{N}\\ \vdots \\ \sin\frac{(N-1)\pi q}{N}-\sin\frac{(N-1)\pi q}{N}\cos\frac{\pi q}{N}\end{pmatrix}\\
&= -\frac{2im}{\hbar\Delta t}(1-\cos\frac{\pi q}{N})w_q,
\end{aligned}$$

so $\lambda_q=-\frac{2im}{\hbar\Delta t}(1-\cos\frac{\pi q}{N})$ with $q=1,\ldots,N-1$. Then, we have

$$\begin{aligned}
\det A &= \prod_{q=1}^{N-1}\lambda_q\\
&= \left(-\frac{2im}{\hbar\Delta t}\right)^{N-1}\prod_{q=1}^{N-1}(1-\cos\frac{\pi q}{N})\\
&= \left(-\frac{im}{\hbar\Delta t}\right)^{N-1}\prod_{q=1}^{N-1}(1-e^{i\frac{\pi}{N}q})(1-e^{-i\frac{\pi}{N}q}) \quad \Leftarrow \text{use } \prod_{q=1}^{N-1}(1-e^{i\frac{\pi}{N}q})(1-e^{-i\frac{\pi}{N}q})=N, \text{ see below}\\
&= \left(-\frac{im}{\hbar\Delta t}\right)^{N-1}N.
\end{aligned}$$

The product $\prod_{q=1}^{N-1}(1-e^{i\frac{\pi}{N}q})(1-e^{-i\frac{\pi}{N}q})$ can be calculated by noticing that $z=e^{\pm i\frac{\pi}{N}q}$ $(q=1,\ldots,N-1)$, together with $z=\pm 1$, are the $2N$ solutions to the polynomial equation $z^{2N}=1$ (fundamental theorem of algebra). Therefore, we have $u^{2N}-1=(u+1)(u-1)\prod_{q=1}^{N-1}[(u-e^{i\frac{\pi}{N}q})(u-e^{-i\frac{\pi}{N}q})]$ (u arbitrary). Dividing both side by $(u+1)(u-1)$ yields an identity

$$\begin{aligned}\prod_{q=1}^{N-1}[(u-e^{i\frac{\pi}{N}q})(u-e^{-i\frac{\pi}{N}q})] &= \frac{u^N-1}{u-1}\frac{u^N+1}{u+1}\\ &= (1+u+u^2+\cdots u^{N-1})\frac{u^N+1}{u+1},\end{aligned}$$

which leads to $\prod_{q=1}^{N-1}[(1-e^{i\frac{\pi}{N}q})(1-e^{-i\frac{\pi}{N}q})]=N$ for $u=1$.

Due to the special form of $y=\frac{im}{\hbar\Delta t}(x_0,0,\ldots,0,x_N)^T$ in (9), it is sufficient for our purpose to work out four matrix entries of A. So we could use the Cramer's rule, $A^{-1}=\frac{1}{\det A}\mathrm{adj}(A)$,

$$\begin{aligned}(A^{-1})_{1,1} &= \frac{1}{\det A}(-1)^{1+1}\left(-\frac{2im}{\hbar\Delta t}\right)^{N-2}\det\begin{pmatrix}1 & -1/2 & & & \\ -1/2 & 1 & -1/2 & & \\ & -1/2 & 1 & & \\ & & & \ddots & -1/2 \\ & & & -1/2 & 1\end{pmatrix}_{(N-2)\times(N-2)}\\ &= \frac{1}{(-\frac{im}{\hbar\Delta t})^{N-1}N}\left(-\frac{im}{\hbar\Delta t}\right)^{N-2}(N-1)\\ &= \frac{i\hbar\Delta t}{m}\frac{N-1}{N},\end{aligned}$$

and similarly, $(A^{-1})_{N-1,N-1}=(A^{-1})_{1,1}$. Furthermore,

$$\begin{aligned}(A^{-1})_{1,N-1} &= \frac{1}{\det A}(-1)^{N-1+1}\left(-\frac{2im}{\hbar\Delta t}\right)^{N-2}\det\begin{pmatrix}-1/2 & & & \\ 1 & -1/2 & & \\ -1/2 & 1 & \ddots & \\ & & \ddots & -1/2\end{pmatrix}_{(N-2)\times(N-2)}\\ &= \frac{1}{(-\frac{im}{\hbar\Delta t})^{N-1}N}(-1)^N\left(-\frac{2im}{\hbar\Delta t}\right)^{N-2}\left(-\frac{1}{2}\right)^{N-2}\\ &= \frac{i\hbar\Delta t}{m}\frac{1}{N},\end{aligned}$$

and $(A^{-1})_{1,N-1}=(A^{-1})_{1,N-1}$.

After substituting these results to (9) and (3), we arrive at

$$\begin{aligned}&G(x',t';x,t)\\ =& \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2}\int\prod_{k=1}^{N-1}dx_k\ \exp\left[\sum_{k=0}^{N-1}\frac{im}{2\hbar\Delta t}(x_{k+1}-x_k)^2\right] \quad \Leftarrow \text{use Eq. (9)}\\ =& \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2}(2\pi)^{(N-1)/2}(\det A)^{-1/2}e^{\frac{1}{2}y^TA^{-1}y}\exp\left[\frac{im}{2\hbar\Delta t}(x_0^2+x_N^2)\right] \quad \Leftarrow \text{use }\det A\text{ and }A^{-1}\\ =& \left(\frac{m}{i\hbar\Delta t}\right)^{N/2}\frac{1}{\sqrt{2\pi}}\left[\left(-\frac{im}{\hbar\Delta t}\right)^{N-1}N\right]^{-1/2}\exp\left[\frac{im}{2\hbar\Delta t}(x_0^2+x_N^2)\right]\\ &\times\exp\left[\frac{1}{2}\left(\tfrac{im}{\hbar\Delta t}x_0\quad \tfrac{im}{\hbar\Delta t}x_N\right)\begin{pmatrix}\frac{i\hbar\Delta t}{m}\frac{N-1}{N} & \frac{i\hbar\Delta t}{m}\frac{1}{N}\\ \frac{i\hbar\Delta t}{m}\frac{1}{N} & \frac{i\hbar\Delta t}{m}\frac{N-1}{N}\end{pmatrix}\begin{pmatrix}\frac{im}{\hbar\Delta t}x_0\\ \frac{im}{\hbar\Delta t}x_N\end{pmatrix}\right]\\ =& \left(\frac{m}{2\pi iN\hbar\Delta t}\right)^{1/2}\exp\left[\frac{im}{2\hbar\Delta t}(x_0^2+x_N^2)\right]\exp\left[\frac{1}{2}\frac{-im}{\hbar\Delta t}\left(\frac{N-1}{N}x_0^2+\frac{2}{N}x_0x_N+\frac{N-1}{N}x_0^2\right)\right]\\ =& \left(\frac{m}{2\pi iN\hbar\Delta t}\right)^{1/2}\exp\left[\frac{1}{2N}\frac{im}{\hbar\Delta t}(x_N-x_0)^2\right] \quad \Leftarrow \text{use } t'-t=N\Delta t\text{ and }x_0=x,\ x_N=x'\\ =& \sqrt{\frac{m}{2\pi i\hbar(t'-t)}}\exp\left[\frac{im(x'-x)^2}{2\hbar(t'-t)}\right],\end{aligned}$$

which indeed agrees with (7) obtained in *Approach 1*.

3. **Partition function for a harmonic oscillator** (3+5 points)

For the harmonic oscillator in one dimension, the Hamiltonian is given by $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$. At finite temperature T, the partition function is define by $Z = \mathrm{Tr}(e^{-\beta\hat{H}})$, where $\beta = 1/T$.

(a) Derive the path integral form of the partition function by dividing the imaginary-time evolution into small time intervals.

(b) Calculate the partition function by performing Gaussian integrations.

Solution: (a) For the partition function, the imaginary-time evolution is divided into N time-slices,

$$\begin{aligned} Z &= \int dx_0\ \langle x_0|e^{-\hat{H}\Delta\tau}\cdots e^{-\hat{H}\Delta\tau}|x_0\rangle \qquad \Leftarrow \text{insert complete basis in coordinate space} \\ &= \int \prod_{k=0}^{N-1} dx_k\ \langle x_0|e^{-\hat{H}\Delta\tau}|x_{N-1}\rangle\langle x_{N-1}|e^{-\hat{H}\Delta\tau}|x_{N-2}\rangle\cdots\langle x_2|e^{-\hat{H}\Delta\tau}|x_1\rangle\langle x_1|e^{-\hat{H}\Delta\tau}|x_0\rangle, \end{aligned} \tag{12}$$

where $N\Delta\tau = \beta$. The propagator for a small time-slice is given by

$$\begin{aligned} &\langle x_{k+1}|e^{-\hat{H}\Delta\tau}|x_k\rangle \\ =\ & \int_{-\infty}^{\infty} dp_k\ \langle x_{k+1}|p_k\rangle\langle p_k|e^{-\hat{H}\Delta\tau}|x_k\rangle \qquad \Leftarrow \text{complete basis in momentum space inserted} \\ \simeq\ & \int_{-\infty}^{\infty} dp_k\ \langle x_{k+1}|p_k\rangle\langle p_k|(1-\hat{H}\Delta\tau)|x_k\rangle \qquad \Leftarrow \text{use } \langle p_k|\hat{H}|x_k\rangle = \left(\frac{p_k^2}{2m} + \frac{1}{2}m\omega^2 x_k^2\right)\langle p_k|x_k\rangle \\ =\ & \int_{-\infty}^{\infty} dp_k\ \left[1 - \left(\frac{p_k^2}{2m} + \frac{1}{2}m\omega^2 x_k^2\right)\Delta\tau\right]\langle x_{k+1}|p_k\rangle\langle p_k|x_k\rangle \\ \simeq\ & \int_{-\infty}^{\infty} \frac{dp_k}{2\pi\hbar}\ e^{-\frac{p_k^2}{2m}\Delta\tau + \frac{i}{\hbar}p_k(x_{k+1}-x_k) - \frac{1}{2}m\omega^2 x_k^2\Delta\tau} \qquad \Leftarrow \text{complete square} \\ =\ & \int_{-\infty}^{\infty} \frac{dp_k}{2\pi\hbar}\ e^{-\frac{\Delta\tau}{2m}[p_k - \frac{im}{\hbar\Delta\tau}(x_{k+1}-x_k)]^2 - \frac{m}{2\hbar^2\Delta\tau}(x_{k+1}-x_k)^2 - \frac{1}{2}m\omega^2 x_k^2\Delta\tau} \quad \Leftarrow \text{Gaussian integral} \\ =\ & \frac{1}{2\pi\hbar}\sqrt{\frac{2m\pi}{\Delta\tau}}e^{-\frac{m}{2\hbar^2\Delta\tau}(x_{k+1}-x_k)^2 - \frac{1}{2}m\omega^2 x_k^2\Delta\tau} \\ =\ & \sqrt{\frac{m}{2\pi\hbar^2\Delta\tau}}e^{-\frac{m}{2\hbar^2\Delta\tau}(x_{k+1}-x_k)^2 - \frac{1}{2}m\omega^2 x_k^2\Delta\tau}. \end{aligned} \tag{13}$$

Substituting this into (12), we obtain

$$Z = \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{N/2}\int\prod_{k=0}^{N-1} dx_k\ e^{-\sum_{k=0}^{N-1}\left[\frac{m}{2\hbar^2\Delta\tau}(x_{k+1}-x_k)^2 + \frac{1}{2}m\omega^2 x_k^2\Delta\tau\right]} \quad \Leftarrow x_N = x_0 \text{ imposed} \tag{14}$$

In the limit $N \to \infty$ and $\Delta\tau \to 0$, we have $x_{k+1} - x_k \to \dot{x}(\tau)\Delta\tau$ and $\Delta\tau\sum_{k=0}^{N-1} \to \int_0^\beta d\tau$, and the partition function is written as a path integral,

$$Z = \int_{x(0)=x(\beta)} \mathcal{D}x(\tau)\ e^{-\int_0^\beta d\tau\left[\frac{m}{2\hbar^2}\dot{x}(\tau)^2 + \frac{1}{2}m\omega^2 x(\tau)^2\right]}.$$

When defining $\tau' \to \tau\hbar$, the path integral is rewritten as

$$\begin{aligned} Z &= \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau')\ e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau'\left[\frac{1}{2}m\dot{x}(\tau')^2 + \frac{1}{2}m\omega^2 x(\tau')^2\right]} \\ &= \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau')\ e^{-S[x(\tau')]/\hbar}, \end{aligned} \tag{15}$$

where $S[x(\tau')] = \int_0^{\beta\hbar} d\tau'\ \left[\frac{1}{2}m\dot{x}(\tau')^2 + \frac{1}{2}m\omega^2 x(\tau')^2\right]$. This completes the derivation of a path integral form for the partition function. Note that (15) is consistent with the result in the lecture note (QM-3.pdf), where in the latter we have set $\hbar = 1$.

(b) In order to keep track of the factors in the integration measure, we evaluate the path integral starting from its discretized version (14). Below we use the multidimensional Gaussian integration formula (8) to calculate the Gaussian integral in (14),

$$\begin{aligned}
&\int \prod_{k=0}^{N-1} dx_k\; e^{-\sum_{k=0}^{N-1}\left[\frac{m}{2\hbar^2\Delta\tau}(x_{k+1}-x_k)^2+\frac{1}{2}m\omega^2 x_k^2\Delta\tau\right]} \\
=\;& \int \prod_{k=0}^{N-1} dx_k\; \exp\left[-\left(\frac{m}{\hbar^2\Delta\tau}+\frac{1}{2}m\omega^2\Delta\tau\right)\sum_{k=0}^{N-1} x_k^2+\frac{m}{\hbar^2\Delta\tau}\sum_{k=0}^{N-1} x_k x_{k+1}\right] \\
=\;& \int \prod_{k=0}^{N-1} dx_k\; e^{-\frac{1}{2}x^T B x} \\
=\;& (2\pi)^{N/2}(\det B)^{-1/2},
\end{aligned} \tag{16}$$

where $x=(x_0,x_1,\ldots,x_{N-1})^T$ and B is given by

$$B=\begin{pmatrix}
\frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau & -\frac{m}{\hbar^2\Delta\tau} & & & -\frac{m}{\hbar^2\Delta\tau} \\
-\frac{m}{\hbar^2\Delta\tau} & \frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau & -\frac{m}{\hbar^2\Delta\tau} & & \\
 & -\frac{m}{\hbar^2\Delta\tau} & \frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau & & \\
 & & & \ddots & -\frac{m}{\hbar^2\Delta\tau} \\
-\frac{m}{\hbar^2\Delta\tau} & & & -\frac{m}{\hbar^2\Delta\tau} & \frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau
\end{pmatrix}_{N\times N}. \tag{17}$$

We note that the form of B is similar to a single-particle Hamiltonian for a 1D tight-binding model with *periodic* boundary condition, whose eigenvectors are plane waves. Having this in mind, the eigenvalue equation for B is given by

$$Bv_q=\lambda_q v_q, \tag{18}$$

where $q=0,1,\ldots,N-1$ and $v_q=\frac{1}{\sqrt{N}}(1,e^{i\frac{2\pi}{N}q},e^{i\frac{2\pi}{N}2q},e^{i\frac{2\pi}{N}3q},\ldots,e^{i\frac{2\pi}{N}(N-1)q})^T$. It is obvious that v_q are orthonormal and complete, $v_q^\dagger v_{q'}=\delta_{qq'}\ \forall q,q'$. Let us verify that they are indeed eigenvectors of B and determine the corresponding eigenvalues λ_q,

$$\begin{aligned}
Bv_q &= \frac{1}{\sqrt{N}}\begin{pmatrix}
\frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau & -\frac{m}{\hbar^2\Delta\tau} & & & -\frac{m}{\hbar^2\Delta\tau} \\
-\frac{m}{\hbar^2\Delta\tau} & \frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau & -\frac{m}{\hbar^2\Delta\tau} & & \\
 & -\frac{m}{\hbar^2\Delta\tau} & \frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau & & \\
 & & & \ddots & -\frac{m}{\hbar^2\Delta\tau} \\
-\frac{m}{\hbar^2\Delta\tau} & & & -\frac{m}{\hbar^2\Delta\tau} & \frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau
\end{pmatrix}\begin{pmatrix} 1 \\ e^{i\frac{2\pi}{N}q} \\ e^{i\frac{2\pi}{N}2q} \\ \vdots \\ e^{i\frac{2\pi}{N}(N-1)q}\end{pmatrix} \\
&= \frac{1}{\sqrt{N}}\begin{pmatrix}
(\frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau)-\frac{m}{\hbar^2\Delta\tau}(e^{i\frac{2\pi}{N}q}+e^{i\frac{2\pi}{N}(N-1)q}) \\
(\frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau)e^{i\frac{2\pi}{N}q}-\frac{m}{\hbar^2\Delta\tau}(1+e^{i\frac{2\pi}{N}2q}) \\
(\frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau)e^{i\frac{2\pi}{N}2q}-\frac{m}{\hbar^2\Delta\tau}(e^{i\frac{2\pi}{N}q}+e^{i\frac{2\pi}{N}3q}) \\
\vdots \\
(\frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau)e^{i\frac{2\pi}{N}(N-1)q}-\frac{m}{\hbar^2\Delta\tau}(1+e^{i\frac{2\pi}{N}(N-2)q})
\end{pmatrix} \\
&= \frac{1}{\sqrt{N}}\left(\frac{2m}{\hbar^2\Delta\tau}+m\omega^2\Delta\tau-\frac{2m}{\hbar^2\Delta\tau}\cos\frac{2\pi q}{N}\right)\begin{pmatrix} 1 \\ e^{i\frac{2\pi}{N}q} \\ e^{i\frac{2\pi}{N}2q} \\ \vdots \\ e^{i\frac{2\pi}{N}(N-1)q}\end{pmatrix} \\
&= \left(\frac{4m}{\hbar^2\Delta\tau}\sin^2\frac{\pi q}{N}+m\omega^2\Delta\tau\right)v_q,
\end{aligned}$$

so $\lambda_q=\frac{4m}{\hbar^2\Delta\tau}\sin^2\frac{\pi q}{N}+m\omega^2\Delta\tau$ with $q=0,1,\ldots,N-1$. Therefore, we have

$$\begin{aligned}
\det B &= \prod_{q=0}^{N-1}\lambda_q \\
&= \prod_{q=0}^{N-1}\left(\frac{4m}{\hbar^2\Delta\tau}\sin^2\frac{\pi q}{N}+m\omega^2\Delta\tau\right),
\end{aligned} \tag{19}$$

and

$$
\begin{aligned}
Z &= \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{N/2} \int \prod_{k=0}^{N-1} dx_k \; e^{-\sum_{k=0}^{N-1}\left[\frac{m}{2\hbar^2\Delta\tau}(x_{k+1}-x_k)^2 + \frac{1}{2}m\omega^2 x_k^2\Delta\tau\right]} \quad \Leftarrow \text{use Eq. (16)} \\
&= \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{N/2} (2\pi)^{N/2} (\det B)^{-1/2} \\
&= \left(\frac{m}{\hbar^2\Delta\tau}\right)^{N/2} \prod_{q=0}^{N-1} \left(\frac{4m}{\hbar^2\Delta\tau}\sin^2\frac{\pi q}{N} + m\omega^2\Delta\tau\right)^{-1/2} \qquad \Leftarrow \Delta\tau = \frac{\beta}{N} \\
&= \left(\frac{N}{\beta\hbar^2}\right)^{N/2} \prod_{q=0}^{N-1} \left(\frac{4N}{\beta\hbar^2}\sin^2\frac{\pi q}{N} + \frac{\beta\omega^2}{N}\right)^{-1/2} \\
&= \prod_{q=0}^{N-1} \left(4\sin^2\frac{\pi q}{N} + \frac{\beta^2\hbar^2\omega^2}{N^2}\right)^{-1/2} \\
&= \frac{N}{\beta\hbar\omega} \prod_{q=1}^{N-1} \left(4\sin^2\frac{\pi q}{N} + \frac{\beta^2\hbar^2\omega^2}{N^2}\right)^{-1/2} \\
&= \frac{N}{\beta\hbar\omega} \frac{\prod_{q=1}^{N-1}\left(1 + \frac{\beta^2\hbar^2\omega^2}{4N^2\sin^2\frac{\pi q}{N}}\right)^{-1/2}}{\prod_{q=1}^{N-1}\left(2\sin\frac{\pi q}{N}\right)} \qquad \Leftarrow \text{use} \prod_{q=1}^{N-1}\left(2\sin\frac{\pi q}{N}\right) = N, \text{ see below} \\
&= \frac{1}{\beta\hbar\omega} \prod_{q=1}^{N-1} \left(1 + \frac{\beta^2\hbar^2\omega^2}{4N^2\sin^2\frac{\pi q}{N}}\right)^{-1/2} . \qquad (20)
\end{aligned}
$$

In obtaining the above results, the product $\prod_{q=1}^{N-1}\left(2\sin\frac{\pi q}{N}\right)$ can be calculated by

$$
\begin{aligned}
\prod_{q=1}^{N-1}\left(2\sin\frac{\pi q}{N}\right) &= \prod_{q=1}^{N-1}\left[(-i)(e^{i\frac{\pi}{N}q} - e^{-i\frac{\pi}{N}q})\right] \\
&= (-i)^{N-1} e^{i\frac{\pi}{N}\sum_{q=1}^{N-1} q} \prod_{q=1}^{N-1}(1 - e^{-i\frac{2\pi}{N}q}) \\
&= (-i)^{N-1} e^{i\frac{\pi}{2}(N-1)} \prod_{q=1}^{N-1}(1 - e^{-i\frac{2\pi}{N}q}) \\
&= \prod_{q=1}^{N-1}(1 - e^{-i\frac{2\pi}{N}q}),
\end{aligned}
$$

and the product $\prod_{q=1}^{N-1}(1 - e^{-i\frac{2\pi}{N}q})$ can be evaluated by noticing that $z = e^{-i\frac{2\pi}{N}q}$ $(q = 1, \ldots, N-1)$, together with $z = 1$, are the N solutions to the polynomial equation $z^N = 1$ (fundamental theorem of algebra). Therefore, we have $u^N - 1 = (u-1)\prod_{q=1}^{N-1}(u - e^{-i\frac{2\pi}{N}q})$ (u arbitrary). Dividing both side by $(u-1)$ yields an identity

$$
\begin{aligned}
\prod_{q=1}^{N-1}(u - e^{-i\frac{2\pi}{N}q}) &= \frac{u^N - 1}{u - 1} \\
&= 1 + u + u^2 + \cdots u^{N-1},
\end{aligned}
$$

which leads to $\prod_{q=1}^{N-1}(1 - e^{-i\frac{2\pi}{N}q}) = N$ for $u = 1$.

In the infinite time-slice limit $N \to \infty$, $N^2\sin^2\frac{\pi q}{N} \to \pi^2 q^2$ for $q \ll N$ and $(N-q) \ll N$, while for other cases $\frac{1}{N^2 \sin^2 \frac{\pi q}{N}} \to 0$. Then, the partition function (20) becomes

$$\begin{aligned}
Z &= \frac{1}{\beta\hbar\omega} \lim_{N\to\infty} \prod_{q=1}^{N-1} \left(1 + \frac{\beta^2\hbar^2\omega^2}{4N^2 \sin^2 \frac{\pi q}{N}}\right)^{-1/2} \\
&= \frac{1}{\beta\hbar\omega} \lim_{N\to\infty} \prod_{1=q\ll N} \left(1 + \frac{\beta^2\hbar^2\omega^2}{4N^2 \sin^2 \frac{\pi q}{N}}\right)^{-1/2} \prod_{1=q\ll N} \left(1 + \frac{\beta^2\hbar^2\omega^2}{4N^2 \sin^2 \frac{\pi(N-q)}{N}}\right)^{-1/2} \\
&= \frac{1}{\beta\hbar\omega} \prod_{q=1}^{\infty} \left(1 + \frac{\beta^2\hbar^2\omega^2}{4\pi^2 q^2}\right)^{-1} \quad \Leftarrow \text{use } \sinh(z) = z \prod_{n=1}^{\infty} \left(1 + \frac{z^2}{n^2\pi^2}\right) \\
&= \frac{1}{\beta\hbar\omega} \frac{\frac{1}{2}\beta\hbar\omega}{\sinh(\frac{1}{2}\beta\hbar\omega)} \\
&= \frac{1}{2\sinh(\frac{1}{2}\beta\hbar\omega)} \\
&= \frac{1}{e^{\frac{1}{2}\beta\hbar\omega} - e^{-\frac{1}{2}\beta\hbar\omega}},
\end{aligned}$$

which is consistent with the derivation based on the bosonic representation (see page 8 in the Lecture note QM-3.pdf).