Quantum Phenomena

1. *One dimensional chain:*

(a) From the Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N-1} \frac{p_i^2}{2m} + \frac{K}{2}\left[u_1^2 + \sum_{i=2}^{N-1}(u_i - u_{i-1})^2 + u_{N-1}^2\right],$$

the classical equations of motion are obtained as

$$m\frac{d^2u_j}{dt^2} = -K(u_j - u_{j-1}) - K(u_j - u_{j+1}) = K(u_{j-1} - 2u_j + u_{j+1}),$$

for $j = 1, 2, \cdots, N-1$, and with $u_0 = u_N = 0$. In a normal mode, the particles oscillate in phase. The usual procedure is to obtain the modes, and corresponding frequencies, by diagonalizing the matrix of coefficeints coupling the displacements on the right hand side of the equation of motion. For any linear system, we have $md^2u_i/dt^2 = \mathcal{K}_{ij}u_j$, and we must diagonalize $\mathcal{K}_{ij}$. In the above example, $\mathcal{K}_{ij}$ is only a function of the difference $i - j$. This is a consequence of translational symmetry, and allows us to diagonalize the matrix using Fourier modes. Due to the boundary conditions in this case, the appropriate transformation involves the sine, and the motion of the j-th particle in a normal mode is given by

$$\tilde{u}_{k(n)}(j) = \sqrt{\frac{2}{N}}e^{\pm i\omega_n t}\sin\left(k(n)\cdot j\right).$$

The origin of time is artibrary, but to ensure that $u_N = 0$, we must set

$$k(n) \equiv \frac{n\pi}{N}, \qquad \text{for} \qquad n = 1, 2, \cdots, N-1.$$

Larger values of n give wave-vectors that are simply shifted by a multiple of π, and hence coincide with one of the above normal modes. The number of normal modes thus equals the number of original displacement variables, as required. Furthermore, the amplitudes are chosen such that the normal modes are also orthonormal, i.e.

$$\sum_{j=1}^{N-1} \tilde{u}_{k(n)}(j)\cdot\tilde{u}_{k(m)}(j) = \delta_{n,m}.$$

By substituting the normal modes into the equations of motion we obtain the dispersion relation

$$\omega_n^2 = 2\omega_0^2 \left[1 - \cos\left(\frac{n\pi}{N}\right)\right] = \omega_0^2 \sin^2\left(\frac{n\pi}{2N}\right),$$

where $\omega_0 \equiv \sqrt{K/m}$.

The potential energy for each normal mode is given by

$$\begin{aligned} U_n &= \frac{K}{2}\sum_{i=1}^{N} |u_i - u_{i-1}|^2 = \frac{K}{N}\sum_{i=1}^{N}\left\{\sin\left(\frac{n\pi}{N}i\right) - \sin\left[\frac{n\pi}{N}(i-1)\right]\right\}^2 \\ &= \frac{4K}{N}\sin^2\left(\frac{n\pi}{2N}\right)\sum_{i=1}^{N}\cos^2\left[\frac{n\pi}{N}\left(i-\frac{1}{2}\right)\right]. \end{aligned}$$

Noting that

$$\sum_{i=1}^{N}\cos^2\left[\frac{n\pi}{N}\left(i-\frac{1}{2}\right)\right] = \frac{1}{2}\sum_{i=1}^{N}\left\{1 + \cos\left[\frac{n\pi}{N}(2i-1)\right]\right\} = \frac{N}{2},$$

we have

$$U_{k(n)} = 2K\sin^2\left(\frac{n\pi}{2N}\right).$$

(b) Before evaluating the classical partition function, lets evaluate the potential energy by first expanding the displacement using the basis of normal modes, as

$$u_j = \sum_{n=1}^{N-1} a_n \cdot \tilde{u}_{k(n)}(j).$$

The expression for the total potential energy is

$$U = \frac{K}{2}\sum_{i=1}^{N}(u_i - u_{i-1})^2 = \frac{K}{2}\sum_{i=1}^{N}\left\{\sum_{n=1}^{N-1} a_n\left[\tilde{u}_{k(n)}(j) - \tilde{u}_{k(n)}(j-1)\right]\right\}^2.$$

Since

$$\sum_{j=1}^{N-1}\tilde{u}_{k(n)}(j)\cdot\tilde{u}_{k(m)}(j-1) = \frac{1}{N}\delta_{n,m}\sum_{j=1}^{N-1}\left\{-\cos\left[k(n)(2j-1)\right] + \cos k(n)\right\} = \delta_{n,m}\cos k(n),$$

the total potential energy has the equivalent forms

$$\begin{aligned} U &= \frac{K}{2}\sum_{i=1}^{N}(u_i - u_{i-1})^2 = K\sum_{n=1}^{N-1} a_n^2\left(1 - \cos k(n)\right), \\ &= \sum_{i=1}^{N-1} a_{k(n)}^2 \varepsilon_{k(n)}^2 = 2K\sum_{i=1}^{N-1} a_{k(n)}^2 \sin^2\left(\frac{n\pi}{2N}\right). \end{aligned}$$

The next step is to change the coordinates of phase space from u_j to a_n. The Jacobian associated with this change of variables is unity, and the classical partition function is now obtained from

$$Z = \frac{1}{\lambda^{N-1}} \int_{-\infty}^{\infty} da_1 \cdots \int_{-\infty}^{\infty} da_{N-1} \exp\left[-2\beta K \sum_{n=1}^{N-1} a_n^2 \sin^2\left(\frac{n\pi}{2N}\right)\right],$$

where $\lambda = h/\sqrt{2\pi m k_B T}$ corresponds to the contribution to the partition function from each momentum coordinate. Performing the Gaussian integrals, we obtain

$$\begin{aligned} Z &= \frac{1}{\lambda^{N-1}} \prod_{n=1}^{N-1} \left\{\int_{-\infty}^{\infty} da_n \exp\left[-2\beta K a_n^2 \sin^2\left(\frac{n\pi}{2N}\right)\right]\right\}, \\ &= \frac{1}{\lambda^{N-1}} \left(\frac{\pi k_B T}{2K}\right)^{\frac{N-1}{2}} \prod_{n=1}^{N-1} \left[\sin\left(\frac{n\pi}{2N}\right)\right]^{-1}. \end{aligned}$$

(c) The average squared amplitude of each normal mode is

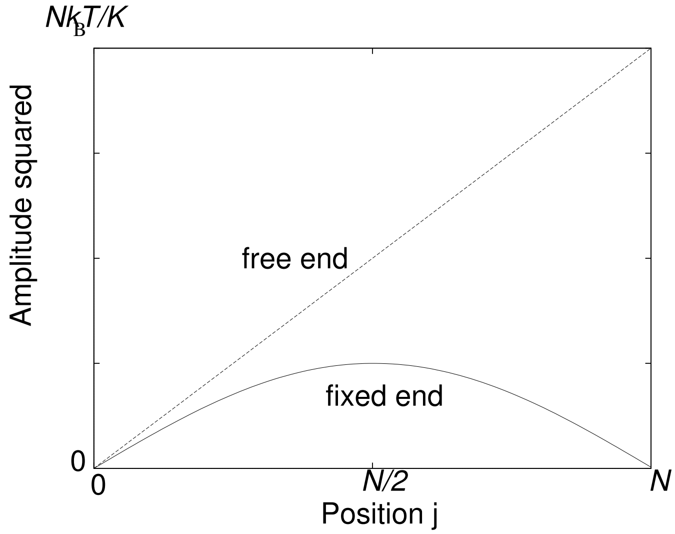
$$\begin{aligned} \left\langle a_n^2 \right\rangle &= \frac{\int_{-\infty}^{\infty} da_n (a_n^2) \exp\left[-2\beta K a_n^2 \sin^2\left(\frac{n\pi}{2N}\right)\right]}{\int_{-\infty}^{\infty} da_n \exp\left[-2\beta K a_n^2 \sin^2\left(\frac{n\pi}{2N}\right)\right]} \\ &= \left[4\beta K \sin^2\left(\frac{n\pi}{2N}\right)\right]^{-1} = \frac{k_B T}{4K} \frac{1}{\sin^2\left(\frac{n\pi}{2N}\right)}. \end{aligned}$$

The variation of the displacement is then given by

$$\begin{aligned} \left\langle u_j^2 \right\rangle &= \left\langle \left[\sum_{n=1}^{N-1} a_n \tilde{u}_n(j)\right]^2 \right\rangle = \sum_{n=1}^{N-1} \left\langle a_n^2 \right\rangle \tilde{u}_n^2(j) \\ &= \frac{2}{N} \sum_{n=1}^{N-1} \left\langle a_n^2 \right\rangle \sin^2\left(\frac{n\pi}{N} j\right) = \frac{k_B T}{2KN} \sum_{n=1}^{N-1} \frac{\sin^2\left(\frac{n\pi}{N} j\right)}{\sin^2\left(\frac{n\pi}{2N}\right)}. \end{aligned}$$

The evaluation of the above sum is considerably simplified by considering the combination

$$\begin{aligned} \left\langle u_{j+1}^2 \right\rangle + \left\langle u_{j-1}^2 \right\rangle - 2\left\langle u_j^2 \right\rangle &= \frac{k_B T}{2KN} \sum_{n=1}^{N-1} \frac{2\cos\left[\frac{2n\pi}{N} j\right] - \cos\left[\frac{2n\pi}{N}(j+1)\right] - \cos\left[\frac{2n\pi}{N}(j-1)\right]}{1 - \cos\left(\frac{n\pi}{N}\right)} \\ &= \frac{k_B T}{2KN} \sum_{n=1}^{N-1} \frac{2\cos\left(\frac{2n\pi}{N} j\right)\left[1 - \cos\left(\frac{n\pi}{N}\right)\right]}{1 - \cos\left(\frac{n\pi}{N}\right)} = -\frac{k_B T}{KN}, \end{aligned}$$



where we have used $\sum_{n=1}^{N-1}\cos(\pi n/N) = -1$. It is easy to check that subject to the boundary conditions of $\langle u_0^2\rangle = \langle u_N^2\rangle = 0$, the solution to the above recursion relation is

$$\langle u_j^2\rangle = \frac{k_BT}{K}\frac{j(N-j)}{N}.$$

(d) When the last particle is free, the overall potential energy is the sum of the contributions of each spring, i.e. $U = K\sum_{j=1}^{N-1}(u_j - u_{j-1})^2/2$. Thus each extension can be treated independently, and we introduce a new set of independent variables $\Delta u_j \equiv u_j - u_{j-1}$. (In the previous case, where the two ends are fixed, these variables were not independent.) The partition function can be calculated separately for each spring as

$$\begin{aligned} Z &= \frac{1}{\lambda^{N-1}}\int_{-\infty}^{\infty} du_1 \cdots \int_{-\infty}^{\infty} du_{N-1}\exp\left[-\frac{K}{2k_BT}\sum_{j=1}^{N-1}(u_j - u_{j-1})^2\right] \\ &= \frac{1}{\lambda^{N-1}}\int_{-\infty}^{\infty} d\Delta u_1 \cdots \int_{-\infty}^{\infty} d\Delta u_{N-1}\exp\left[-\frac{K}{2k_BT}\sum_{j=1}^{N-1}\Delta u_j^2\right] = \left(\frac{2\pi k_BT}{\lambda^2 K}\right)^{(N-1)/2}. \end{aligned}$$

For each spring extension, we have

$$\langle \Delta u_j^2\rangle = \langle (u_j - u_{j-1})^2\rangle = \frac{k_BT}{K}.$$

The displacement

$$u_j = \sum_{i=1}^{j}\Delta u_i,$$

is a sum of *independent* random variables, leading to the variance

$$\left\langle u_j^2 \right\rangle = \left\langle \left(\sum_{i=1}^{j} \Delta u_i \right)^2 \right\rangle = \sum_{i=1}^{j} \left(\Delta u_i\right)^2 = \frac{k_B T}{K} j.$$

The results for displacements of open and closed chains are compared in the above figure.

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2. *Black Hole Thermodynamics:* The (quantum) vacuum undergoes fluctuations in which particle–antiparticle pairs are constantly created and destroyed. Near the boundary of a black hole, sometimes one member of a pair falls into the black hole while the other escapes. This is a hand-waving explanation for the emission of radiation from black holes.

(a) The classical escape velocity is obtained by equating the gravitational energy and the kinetic energy on the surface as,

$$G\frac{Mm}{R} = \frac{mv_E^2}{2},$$

leading to

$$v_E = \sqrt{\frac{2GM}{r}}.$$

Setting the escape velocity to the speed of light, we find

$$R = \frac{2G}{c^2}M.$$

For a mass larger than given by this ratio (i.e. $M > c^2 R/2G$), nothing will escape from distances closer than R.

(b) When two black holes of mass M collapse into one, the entropy change is

$$\begin{aligned}\Delta S = S_2 - 2S_1 &= \frac{k_B c^3}{4G\hbar}\left(A_2 - 2A_1\right) = \frac{k_B c^3}{4G\hbar} 4\pi \left(R_2^2 - 2R_1^2\right)\\ &= \frac{\pi k_B c^3}{G\hbar}\left[\left(\frac{2G}{c^2}2M\right)^2 - 2\left(\frac{2G}{c^2}M\right)^2\right] = \frac{8\pi G k_B M^2}{c\hbar} > 0.\end{aligned}$$

Thus the merging of black holes increases the entropy of the universe.

Consider the coalescence of two solar mass black holes. The entropy change is

$$\begin{aligned}\Delta S &= \frac{8\pi G k_B M_\odot^2}{c\hbar}\\ &\approx \frac{8\pi \cdot 6.7 \times 10^{-11}(N \cdot m^2/kg^2) \cdot 1.38 \times 10^{-23}(J/K) \cdot (2 \times 10^{30})^2 kg^2}{3 \times 10^8 (m/s) \cdot 1.05 \times 10^{-34}(J \cdot s)}\\ &\approx 3 \times 10^{54}(J/K).\end{aligned}$$

In units of bits, the information lost is

$$N_I = \frac{\Delta S \ln 2}{k_B} = 1.5 \times 10^{77}.$$

(c) Using the thermodynamic definition of temperature $\frac{1}{T} = \frac{\partial S}{\partial E}$, and the Einstein relation $E = Mc^2$,

$$\frac{1}{T} = \frac{1}{c^2}\frac{\partial}{\partial M}\left[\frac{k_B c^3}{4G\hbar} 4\pi \left(\frac{2G}{c^2}M\right)^2\right] = \frac{8\pi k_B G}{\hbar c^3} M, \qquad \Longrightarrow \qquad T = \frac{\hbar c^3}{8\pi k_B G}\frac{1}{M}.$$

(d) The decrease in energy E of a black body of area A at temperature T is given by the Stefan-Boltzmann law,

$$\frac{1}{A}\frac{\partial E}{\partial t} = -\sigma T^4, \quad \text{where} \quad \sigma = \frac{\pi^2 k_B^4}{60\hbar^3 c^2}.$$

(e) Using the result in part (d) we can calculate the time it takes a black hole to evaporate. For a black hole

$$A = 4\pi R^2 = 4\pi \left(\frac{2G}{c^2}M\right)^2 = \frac{16\pi G^2}{c^4}M^2, \quad E = Mc^2, \quad \text{and} \quad T = \frac{\hbar c^3}{8\pi k_B G}\frac{1}{M}.$$

Hence

$$\frac{d}{dt}\left(Mc^2\right) = -\frac{\pi^2 k_B^4}{60\hbar^3 c^2}\left(\frac{16\pi G^2}{c^4}M^2\right)\left(\frac{\hbar c^3}{8\pi k_B G}\frac{1}{M}\right)^4,$$

which implies that

$$M^2 \frac{dM}{dt} = -\frac{\hbar c^4}{15360 G^2} \equiv -b.$$

This can be solved to give

$$M(t) = \left(M_0^3 - 3bt\right)^{1/3}.$$

The mass goes to zero, and the black hole evaporates after a time

$$\tau = \frac{M_0^3}{3b} = \frac{5120 G^2 M\odot^3}{\hbar c^4} \approx 2.2 \times 10^{74} s,$$

which is considerably longer than the current age of the universe (approximately $\times 10^{18} s$).

(f) The temperature and mass of a black hole are related by $M = \hbar c^3/(8\pi k_B G T)$. For a black hole in thermal equilibrium with the current cosmic background radiation at $T = 2.7°K$,

$$M \approx \frac{1.05 \times 10^{-34}(J \cdot s)(3 \times 10^8)^3 (m/s)^3}{8\pi \cdot 1.38 \times 10^{-23}(J/K) \cdot 6.7 \times 10^{-11}(N \cdot m^2/kg^2) \cdot 2.7°K} \approx 4.5 \times 10^{22} kg.$$

(g) The mass inside the spherical volume of radius R must be less than the mass that would make a black hole that fills this volume. Bring in additional mass (from infinity) inside the volume, so as to make a volume-filling balck hole. Clearly the entropy of the system will increase in the process, and the final entropy, which is the entropy of the black hole is larger than the initial entropy in the volume, leading to the inequality

$$S \leq S_{BH} = \frac{k_B c^3}{4G\hbar} A,$$

where $A = 4\pi R^2$ is the area enclosing the volume. The surprising observation is that the upper bound on the entropy is proportional to area, whereas for any system of particles we expect the entropy to be proportional to N. This should remain valid even at very high temperatures when interactions are unimportant. The 'holographic principle' is an allusion to the observation that it appears as if the degrees of freedom are living on the surface of the system, rather than its volume. It was formulated in the context of string theory which attempts to construct a consistent theory of quantum gravity, which replaces particles as degrees of freedom, with strings.

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3. *Quantum Oscillator:*

(a) The partition function Z, at a temperature T, is given by

$$Z = \mathrm{tr}\,\rho = \sum_n e^{-\beta E_n}.$$

As the energy levels for a harmonic oscillator are given by

$$\epsilon_n = \hbar\omega\left(n + \frac{1}{2}\right),$$

the partition function is

$$\begin{aligned} Z &= \sum_n \exp\left[-\beta\hbar\omega\left(n + \frac{1}{2}\right)\right] = e^{-\beta\hbar\omega/2} + e^{-3\beta\hbar\omega/2} + \cdots \\ &= \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}} = \frac{1}{2\sinh\left(\beta\hbar\omega/2\right)}. \end{aligned}$$

The expectation value of the energy is

$$\langle\mathcal{H}\rangle = -\frac{\partial \ln Z}{\partial\beta} = \left(\frac{\hbar\omega}{2}\right)\frac{\cosh(\beta\hbar\omega/2)}{\sinh(\beta\hbar\omega/2)} = \left(\frac{\hbar\omega}{2}\right)\frac{1}{\tanh(\beta\hbar\omega/2)}.$$

(b) Using the formal representation of the energy eigenstates, the density matrix ρ is

$$\rho = 2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\left(\sum_n |n > \exp\left[-\beta\hbar\omega\left(n+\frac{1}{2}\right)\right] < n|\right).$$

In the coordinate representation, the eigenfunctions are in fact given by

$$\langle n|q\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{H_n(\xi)}{\sqrt{2^n n!}}\exp\left(-\frac{\xi^2}{2}\right),$$

where

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}q,$$

with

$$\begin{aligned} H_n(\xi) &= (-1)^n \exp(\xi^2)\left(\frac{d}{d\xi}\right)^n \exp(-\xi^2) \\ &= \frac{\exp(\xi^2)}{\pi}\int_{-\infty}^{\infty}(-2iu)^n \exp(-u^2+2i\xi u)du. \end{aligned}$$

For example,

$$H_0(\xi) = 1, \qquad \text{and} \qquad H_1(\xi) = -\exp(\xi^2)\frac{d}{d\xi}\exp(-\xi^2) = 2\xi,$$

result in the eigenstates

$$\langle 0|q\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}q^2\right),$$

and

$$\langle 1|q\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}q\cdot\exp\left(-\frac{m\omega}{2\hbar}q^2\right).$$

Using the above expressions, the matrix elements are obtained as

$$\begin{aligned} \langle q'|\rho|q\rangle &= \sum_{n,n'}\langle q'|n'\rangle\langle n'|\rho|n\rangle\langle n|q\rangle = \frac{\sum_n \exp\left[-\beta\hbar\omega\left(n+\frac{1}{2}\right)\right]\cdot\langle q'|n\rangle\langle n|q\rangle}{\sum_n \exp\left[-\beta\hbar\omega\left(n+\frac{1}{2}\right)\right]} \\ &= 2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\cdot\sum_n \exp\left[-\beta\hbar\omega\left(n+\frac{1}{2}\right)\right]\cdot\langle q'|n\rangle\langle n|q\rangle. \end{aligned}$$

(c) By definition

$$e^A = \sum_{n=0}^{\infty}\frac{1}{n!}A^n,$$

and

$$\frac{\partial e^A}{\partial x} = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial A^n}{\partial x}.$$

But for a product of n operators,

$$\frac{\partial}{\partial x}(A \cdot A \cdots A) = \frac{\partial A}{\partial x} \cdot A \cdots A + A \cdot \frac{\partial A}{\partial x} \cdots A + \cdots + A \cdot A \cdots \frac{\partial A}{\partial x}.$$

The $\frac{\partial A}{\partial x}$ can be moved through the $A's$ surrounding it only if $\left[A, \frac{\partial A}{\partial x}\right] = 0$, in which case

$$\frac{\partial A}{\partial x} = n \frac{\partial A}{\partial x} A^{n-1}, \qquad \text{and} \qquad \frac{\partial e^A}{\partial x} = \frac{\partial A}{\partial x} e^A.$$

However, as we can always reorder operators inside a trace, i.e. $\mathrm{tr}(BC) = \mathrm{tr}(CB)$, and

$$\mathrm{tr}\left(A \cdots A \cdots \frac{\partial A}{\partial x} \cdots A\right) = \mathrm{tr}\left(\frac{\partial A}{\partial x} \cdot A^{n-1}\right),$$

and the identity

$$\frac{\partial}{\partial x} \mathrm{tr}\left(e^A\right) = \mathrm{tr}\left(\frac{\partial A}{\partial x} \cdot e^A\right),$$

can always be satisfied, independent of any constraint on $\left[A, \frac{\partial A}{\partial x}\right]$.

(d) The expectation values of the kinetic and potential energy are given by

$$\left\langle \frac{p^2}{2m} \right\rangle = \mathrm{tr}\left(\frac{p^2}{2m}\rho\right), \qquad \text{and} \qquad \left\langle \frac{m\omega^2 q^2}{2} \right\rangle = \mathrm{tr}\left(\frac{m\omega^2 q^2}{2}\rho\right).$$

Noting that the expression for the partition function derived in part (a) is independent of mass, we know that $\partial Z/\partial m = 0$. Starting with $Z = \mathrm{tr}\left(e^{-\beta\mathcal{H}}\right)$, and differentiating

$$\frac{\partial Z}{\partial m} = \frac{\partial}{\partial m} \mathrm{tr}\left(e^{-\beta\mathcal{H}}\right) = \mathrm{tr}\left[\frac{\partial}{\partial m}(-\beta\mathcal{H})e^{-\beta\mathcal{H}}\right] = 0,$$

where we have used the result in part (c). Differentiating the Hamiltonian, we find that

$$\mathrm{tr}\left[\beta\frac{p^2}{2m^2}e^{-\beta\mathcal{H}}\right] + \mathrm{tr}\left[-\beta\frac{m\omega^2 q^2}{2}e^{-\beta\mathcal{H}}\right] = 0.$$

Equivalently,

$$\mathrm{tr}\left[\frac{p^2}{2m}e^{-\beta\mathcal{H}}\right] = \mathrm{tr}\left[\frac{m\omega^2 q^2}{2}e^{-\beta\mathcal{H}}\right],$$

which shows that the expectation values of kinetic and potential energies are equal.

(e) In part (a) it was found that $\langle\mathcal{H}\rangle = (\hbar\omega/2)\left(\tanh(\beta\hbar\omega/2)\right)^{-1}$. Note that $\langle\mathcal{H}\rangle = \left\langle p^2/2m\right\rangle + \left\langle m\omega^2 q^2/2\right\rangle$, and that in part (d) it was determined that the contribution from the kinetic and potential energy terms are equal. Hence,

$$\left\langle m\omega^2 q^2/2\right\rangle = \frac{1}{2}\left(\hbar\omega/2\right)\left(\tanh(\beta\hbar\omega/2)\right)^{-1}.$$

Solving for $\left\langle q^2\right\rangle$,

$$\left\langle q^2\right\rangle = \frac{\hbar}{2m\omega}\left(\tanh(\beta\hbar\omega/2)\right)^{-1} = \frac{\hbar}{2m\omega}\coth(\beta\hbar\omega/2).$$

While the classical result $\left\langle q^2\right\rangle = k_B T/m\omega^2$, vanishes as $T \to 0$, the quantum result saturates at $T = 0$ to a constant value of $\left\langle q^2\right\rangle = \hbar/(2m\omega)$. The amplitude of the displacement curves in Problem 1 are effected by exactly the same saturation factors.

(f) Using the general operator identity

$$\exp(\beta A)\exp(\beta B) = \exp\left[\beta(A+B) + \beta^2[A,B]/2 + \mathcal{O}(\beta^3)\right],$$

the Boltzmann operator can be decomposed in the high temperature limit into those for kinetic and potential energy; to the lowest order as

$$\exp\left(-\beta\frac{p^2}{2m} - \beta\frac{m\omega^2 q^2}{2}\right) \approx \exp(-\beta p^2/2m)\cdot\exp(-\beta m\omega^2 q^2/2).$$

The first term is the Boltzmann operator for an ideal gas. The second term contains an operator diagonalized by $|q>$. The density matrix element

$$\begin{aligned} < q'|\rho|q> &=< q'|\exp(-\beta p^2/2m)\exp(-\beta m\omega^2 q^2/2)|q> \\ &= \int dp' < q'|\exp(-\beta p^2/2m)|p'>< p'|\exp(-\beta m\omega^2 q^2/2)|q> \\ &= \int dp' < q'|p'>< p'|q>\exp(-\beta p'^2/2m)\exp(-\beta q^2 m\omega^2/2). \end{aligned}$$

Using the free particle basis $< q'|p'>= \frac{1}{\sqrt{2\pi\hbar}}e^{-iq\cdot p/\hbar}$,

$$< q'|\rho|q>= \frac{1}{2\pi\hbar}\int dp' e^{ip'(q-q')/\hbar}e^{-\beta p'^2/2m}e^{-\beta q^2 m\omega^2/2}$$

$$= e^{-\beta q^2 m\omega^2/2}\frac{1}{2\pi\hbar}\int dp'\exp\left[-\left(p'\sqrt{\frac{\beta}{2m}} + \frac{i}{2\hbar}\sqrt{\frac{2m}{\beta}}(q-q')\right)^2\right]\exp\left(-\frac{1}{4}\frac{2m}{\beta\hbar^2}(q-q')^2\right),$$

where we completed the square. Hence

$$< q'|\rho|q >= \frac{1}{2\pi\hbar} e^{-\beta q^2 m\omega^2/2} \sqrt{2\pi m k_B T} \exp\left[-\frac{m k_B T}{2\hbar^2} (q - q')^2 \right].$$

The proper normalization in the high temperature limit is

$$\begin{aligned} Z &= \int dq < q|e^{-\beta p^2/2m} \cdot e^{-\beta m\omega^2 q^2/2}|q > \\ &= \int dq \int dp' < q|e^{-\beta p^2/2m}|p' >< p'|e^{-\beta m\omega^2 q^2/2}|q > \\ &= \int dq \int dp \,|< q|p >|^2 \, e^{-\beta p'^2/2m} e^{-\beta m\omega^2 q^2/2} = \frac{k_B T}{\hbar\omega}. \end{aligned}$$

Hence the properly normalized matrix element in the high temperature limit is

$$< q'|\rho|q >_{\lim T\to\infty} = \sqrt{\frac{m\omega^2}{2\pi k_B T}} \exp\left(-\frac{m\omega^2}{2k_B T} q^2 \right) \exp\left[-\frac{m k_B T}{2\hbar^2} (q - q')^2 \right].$$

(g) In the low temperature limit, we retain only the first terms in the summation

$$\rho_{\lim T\to 0} \approx \frac{|0 > e^{-\beta\hbar\omega/2} < 0| + |1 > e^{-3\beta\hbar\omega/2} < 1| + \cdots}{e^{-\beta\hbar\omega/2} + e^{-3\beta\hbar\omega/2}}.$$

Retaining only the term for the ground state in the numerator, but evaluating the geometric series in the denominator,

$$< q'|\rho|q >_{\lim T\to 0} \approx < q'|0 >< 0|q > e^{-\beta\hbar\omega/2} \cdot \left(e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2} \right).$$

Using the expression for $< q|0 >$ given in part (b),

$$< q'|\rho|q >_{\lim T\to 0} \approx \sqrt{\frac{m\omega}{\pi\hbar}} \exp\left[-\frac{m\omega}{2\hbar} \left(q^2 + q'^2 \right) \right] \left(1 - e^{-\beta\hbar\omega} \right).$$

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