DYLAN J. TEMPLES: Solution Set Four

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1 Shankar 7.3.6.

Consider a particle of mass m in a potential

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2, & x > 0\\ \infty, & x \le 0 \end{cases}$$
(1)

The boundary condition on the wave function is such that $\psi(x = 0) = 0$. The derivative does not need to be continuous because the potential is discontinuous and jumps to infinity at x = 0. The solutions to the whole harmonic oscillator are Gaussians multiplied by a polynomial in x. The normalization factor of any energy eigenfunction is completely determined by two numbers, c_0 for even-n states and c_1 for odd-n states. It is important to note that the Hermite polynomials for odd-n are odd functions and for even-n, they are even functions. For odd-n states the boundary condition is always satisfied because odd functions are zero at x = 0. However, for even-n states, the value of $\psi(x = 0)$ is completely determined by the normalization constant c_0 . This must be zero for the wave function to satisfy the boundary condition. If the first even coefficient is zero, then due to the recursion relation all subsequent even eigenstates must be zero as well. This implies that the half harmonic oscillator can only have odd-n states. For these states, the form of the eigenfunction is the same, but the normalization factor must be adjusted to reflect normalization over $0 < x < \infty$ instead of all x-space. The normalization condition is

$$1 = \int_{-\infty}^{\infty} |\psi_{HO}|^2 dx = 2 \int_{0}^{\infty} |\psi_{HO}|^2 dx , \qquad (2)$$

because the integrand is not negative anywhere in all space. The new wave function must only differ from the harmonic oscillator wave function ψ_{HO} by a constant, so the normalization condition for the half-harmonic oscillator is

$$1 = \int_0^\infty |\psi_{HHO}|^2 dx = \int_0^\infty |a|^2 |\psi_{HO}|^2 dx , \qquad (3)$$

substituting in the normalization condition for the full harmonic oscillator yields

$$2\int_0^\infty |\psi_{HO}|^2 dx = |a|^2 \int_0^\infty |\psi_{HO}|^2 dx , \qquad (4)$$

so that $a = \sqrt{2}$ and $\psi_{HHO} = \sqrt{2}\psi_{HO}$. The eigenfunctions for the half harmonic oscillator are then

$$\psi_{HHO} = \sqrt{2} \left[\frac{m\omega}{\pi \hbar 2^{2n} (n!)^2} \right]^{1/4} \exp\left[-\frac{m\omega x^2}{2\hbar} \right] H_n \left[\left(\frac{m\omega}{\hbar} \right)^{1/2} x \right] \qquad n = 1, 3, 5, \dots$$
(5)

The new factor attached to the eigenfunction will cancel when plugged into the Schr'odinger equation, so the energy spectrum (eigenvalues) will not change. It is the same as the full harmonic oscillator with only odd-n allowed,

$$E_n = (n + \frac{1}{2})\hbar\omega . (6)$$

2 Shankar 7.5.4.

The Boltzman formula

$$P(i) = e^{-\beta E(i)} / Z , \qquad (7)$$

where

$$Z = \sum_{i} e^{-\beta E(i)} \tag{8}$$

gives the probability of finding a system in a state *i* with energy E(i), when it is in thermal equilibrium with a reservoir of absolute temperature $T = 1/\beta k$, with $k = 1.4 \times 10^{-6}$ ergs/K; being Boltzman's constant. (The "probability" referred to above is in relation to a classical ensemble of similar systems and has nothing to do with quantum mechanics.)

2.1 Thermal Average of System's Energy.

The thermal average of the systems energy is given by

$$\bar{E} = -\frac{\partial}{\partial\beta} \ln Z \ . \tag{9}$$

Plugging in the partition function yields

$$\bar{E} = -\frac{\partial}{\partial\beta} \ln\left[\sum_{i} e^{-\beta E(i)}\right] , \qquad (10)$$

using the chain rule to get the derivative gives

$$\bar{E} = -\frac{1}{\sum_{i} e^{-\beta E(i)}} [-E(i)] e^{-\beta E(i)} = E(i) \frac{e^{-\beta E(i)}}{Z} = E(i)P(i) .$$
(11)

2.2 Classical Oscillator.

Let the system be a classical oscillator. The index *i* is now continuous and corresponds to the variables *x* and *p* describing the state of the oscillator, i.e., $i \to x, p$, and $\sum_i \to \int \int dx dp$, and

$$E(i) \to E(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$
 (12)

With these transformations, the partition function becomes

$$Z_{cl} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx \, dp \, e^{-\beta E(x,p)} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx \, dp \, \exp\left[-\beta \frac{p^2}{2m} - \beta \frac{1}{2}m\omega^2 x^2\right]$$
(13)

$$= \int_{-\infty}^{\infty} \exp\left[-\beta \frac{1}{2}m\omega^2 x^2\right] dx \int_{-\infty}^{\infty} \exp\left[-\beta \frac{p^2}{2m}\right] dp$$
(14)

$$=\sqrt{\frac{2\pi}{m\beta\omega^2}}\sqrt{\frac{2\pi m}{\beta}} = \frac{2\pi}{\beta\omega} , \qquad (15)$$

and the thermal average energy becomes

$$\bar{E}_{cl} = -\frac{\partial}{\partial\beta} \ln Z_{cl} = -\frac{1}{Z_{cl}} \frac{\partial}{\partial\beta} Z_{cl} = -\frac{\beta\omega}{2\pi} \frac{(-2\pi)}{\omega\beta^2} = \frac{1}{\beta} = \frac{1}{kT}.$$
(16)

2.3 Quantum Oscillator.

The energy of a quantum harmonic oscillator in state n is $E_n = (n + \frac{1}{2})\hbar\omega$. Thus the quantum partition function is

$$Z_{qu} = \sum_{n=0}^{\infty} e^{-\beta(n+\frac{1}{2})\hbar\omega} = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} e^{-\beta n\hbar\omega} = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} \frac{1}{e^{\beta n\hbar\omega}} = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} \frac{1}{A^n} , \qquad (17)$$

where $A = \exp(\beta \hbar \omega)$. The final sum converges to $1/(1 - A^{-1})$, so the partition function becomes

$$Z_{qu} = e^{-\beta\hbar\omega/2} \frac{1}{1 - A^{-1}} = e^{-\beta\hbar\omega/2} (1 - e^{-\beta\hbar\omega})^{-1} .$$
(18)

The quantum average thermal energy is

$$\bar{E}_{qu} = -\frac{\partial}{\partial\beta} \ln Z_{qu} = -\frac{1}{Z_{qu}} \frac{\partial}{\partial\beta} Z_{qu} = -\frac{1}{Z_{qu}} \frac{\partial}{\partial\beta} e^{-\beta\hbar\omega/2} (1 - e^{-\beta\hbar\omega})^{-1}$$
(19)

$$= -\frac{1}{Z_{qu}} \left[(-\hbar\omega/2) \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} + e^{-\beta\hbar\omega/2} \frac{(-1)\omega\hbar e^{\beta\omega\hbar}}{(1 - e^{-\beta\hbar\omega})^2} \right]$$
(20)

$$= -\frac{1}{Z_{qu}} \left[-\frac{\hbar\omega}{2} Z_{qu} + e^{-\beta\hbar\omega/2} \frac{(-1)\omega\hbar e^{\beta\omega\hbar}}{(1-e^{-\beta\hbar\omega})^2} \right]$$
(21)

$$= -\frac{1}{Z_{qu}} \left[-\frac{\hbar\omega}{2} Z_{qu} - Z_{qu} \frac{\omega\hbar e^{\beta\omega\hbar}}{(1 - e^{-\beta\hbar\omega})} \right]$$
(22)

$$=\hbar\omega\left[\frac{1}{2} + \frac{e^{\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}}\right] = \hbar\omega\left[\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1}\right]$$
(23)

2.4 Large *T* Limit.

It is intuitively clear that as the temperature T increases (and $\beta = 1/kT$ decreases) the oscillator will get more and more excited and eventually (from the correspondence principle) $\bar{E}_{qu} \to \bar{E}_{cl}$ as $T \to \infty$. As β drops the exponential term becomes closer to one, the Taylor series representation of the exponential, to first order is $e^x \simeq 1 + x$. This makes the quantum average thermal energy

$$\bar{E}_{qu} \simeq \hbar\omega \left[\frac{1}{2} + \frac{1}{1 + \beta\hbar\omega - 1} \right] = \hbar\omega \left[\frac{\beta\hbar\omega}{2\beta\hbar\omega} + \frac{2}{2\beta\hbar\omega} \right] , \qquad (24)$$

in the limit $T \to \infty$, $\beta \to 0$, so $2 \gg \beta \hbar \omega$, so the average thermal energy becomes

$$\bar{E}_{qu} \simeq \hbar \omega \frac{2}{2\beta \hbar \omega} = \frac{1}{\beta} = \bar{E}_{cl} \ . \tag{25}$$

Specifically, in this limit "large T" means $T \gg \hbar \omega/k$, because in order to expand the exponential, the argument must be small, which occurs for the condition stated.

2.5 Crystal Structure.

Consider a crystal with N_0 atoms, which for small oscillations, is equivalent to $3N_0$ decoupled oscillators. The mean thermal energy of the crystal $\bar{E}_{crystal}$ is \bar{E}_{qu} or \bar{E}_{cl} summed over all the normal modes. If the oscillators are treated classically, the specific heat per atom is

$$C_{cl}(T) = \frac{1}{N_0} \frac{\partial E_{crystal}}{\partial T} .$$
(26)

The classical energy of the crystal is given by $\bar{E}_{crystal} = 3N_0\bar{E}_{cl}$, the specific heat per atom, classically is then,

$$C_{cl}(T) = \frac{1}{N_0} \frac{\partial}{\partial T} 3N_0 \bar{E}_{cl} = 3k \frac{\partial}{\partial T} T = 3k , \qquad (27)$$

which is independent of T and the parameters of the oscillators and hence the same for all crystals whose atoms behave as point particles with no internal degrees of freedom. This agrees with experiment at high temperatures but not as $T \rightarrow 0$. Empirically,

$$C(T) \to \begin{cases} 3k & (T \text{ large}) \\ 0 & (T \to 0) \end{cases}$$
 (28)

When the oscillators are treated quantum mechanically, as Einstein did, and assuming for simplicity that they all have the same frequency ω , the specific heat per atom is

$$C_{cl}(T) = \frac{1}{N_0} \frac{\partial}{\partial T} 3N_0 \hbar \omega \left[\frac{1}{2} + \frac{1}{e^{\beta \hbar \omega} - 1} \right] = 3\hbar \omega \frac{\partial}{\partial T} (e^{\hbar \omega / kT} - 1)^{-1}$$
(29)

$$=3\hbar\omega\left[(-1)(e^{\hbar\omega/kT}-1)^{-2}\frac{\hbar\omega}{k}(-T^{-2})e^{\hbar\omega/kT}\right]\left(\frac{k}{k}\right)$$
(30)

$$= 3k \left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT} - 1)^2} = 3k \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2} , \qquad (31)$$

where $\theta_E = \hbar \omega / k$ is called the Einstein temperature and varies from crystal to crystal.

The high temperature limit, $T \gg \theta_E$, reduces to the classical specific heat,

$$\lim_{\theta_E/T \ll 1} 3k \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2} = 3k \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2} , \qquad (32)$$

for small $\tau = \theta_E/T$, the exponentials can be expanded in a first order Taylor series,

$$3k\tau^2 \frac{1+\tau}{(1+\tau-1)^2} = 3k(1+\tau) \simeq 3k , \qquad (33)$$

because τ is negligible compared to one. The high temperature limit of the quantum mechanical specific heat per atom reduces to the classical value.

The low temperature limit, $T \ll \theta_E$, so

$$\lim_{\theta_E/T\gg 1} 3k \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2} = 3k \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T})^2} = 3k \left(\frac{\theta_E}{T}\right)^2 e^{-\theta_E/T} .$$
 (34)

Although $C_{qu}(T) \to 0$, the exponential falloff disagrees with the observed $C(T) \to_{T\to 0} T^3$ behavior. This discrepancy arises from assuming that the frequencies of all normal modes are equal, which is of course not generally true. [Recall that in the case of two coupled masses we get $\omega_I = \sqrt{k/m}$ and $\omega_{II} = \sqrt{3k/m}$.] This discrepancy was eliminated by Debye.

3 Problem #3: Matrix Hamiltonians

3.1 Functional Forms of Operators.

Consider the operators A and A^{\dagger} :

$$A = \frac{d}{dx} + W(x), \qquad A^{\dagger} = -\frac{d}{dx} + W(x) .$$
 (35)

For specific forms of W(x), these operators will satisfy the commutation relations for the raising and lowering operators of the quantum harmonic oscillator. The commutation relation for the harmonic oscillator raising and lowering operators is $[a, a^{\dagger}] = 1$, so for these operators

$$AA^{\dagger} = \left(\frac{d}{dx} + W(x)\right)\left(-\frac{d}{dx} + W(x)\right) = -\frac{d}{dx^2} - W(x)\frac{d}{dx} + \frac{d}{dx}W(x) + W(x)^2 , \qquad (36)$$

these are all operators, so the third term is a chain rule. Consider the third term acting on a function $\zeta(x)$,

$$\frac{d}{dx}W(x)\zeta(x) = \zeta(x)\frac{d}{dx}W(x) + W(x)\frac{d}{dx}\zeta(x),$$
(37)

using this operator property, Equation 36 becomes

$$AA^{\dagger} = -\frac{d}{dx^2} - W(x)\frac{d}{dx} + \frac{d}{dx}W(x) + W(x)\frac{d}{dx} + W(x)^2 = -\frac{d}{dx^2} + \frac{d}{dx}W(x) + W(x)^2 .$$
(38)

The other half of the commutator $[A, A^{\dagger}]$ is

$$A^{\dagger}A = \left(-\frac{d}{dx} + W(x)\right)\left(\frac{d}{dx} + W(x)\right) = -\frac{d}{dx^2} + W(x)\frac{d}{dx} - \frac{d}{dx}W(x) + W(x)^2 , \qquad (39)$$

which, using Equation 37, becomes

$$A^{\dagger}A = -\frac{d}{dx^2} + W(x)\frac{d}{dx} - \frac{d}{dx}W(x) - W(x)\frac{d}{dx} + W(x)^2 = -\frac{d}{dx^2} - \frac{d}{dx}W(x) + W(x)^2 .$$
(40)

The commutator is then

$$[A, A^{\dagger}] = \left(-\frac{d}{dx^2} + \frac{d}{dx}W(x) + W(x)^2\right) - \left(-\frac{d}{dx^2} - \frac{d}{dx}W(x) + W(x)^2\right) = 2\frac{d}{dx}W(x) = 1 , \quad (41)$$

so the form of W(x) can be found by solving

$$W'(x) = \frac{1}{2} \qquad \Rightarrow \qquad W(x) = \frac{x}{2} + \alpha , \qquad (42)$$

where α is an arbitrary constant, which will be set to zero. Now the other commutation relations can be verified for this for of W(x), $[a, a] = [a^{\dagger}, a^{a^{\dagger}}] = 0$,

$$[A,A] = \left(-\frac{d^2}{d^2x} - \frac{d}{dx}\frac{x}{2} - \frac{x}{2}\frac{d}{dx} + \frac{x^2}{4}\right) - \left(-\frac{d^2}{d^2x} - \frac{d}{dx}\frac{x}{2} - \frac{x}{2}\frac{d}{dx} + \frac{x^2}{4}\right) = 0$$
(43)

$$[A^{\dagger}, A^{\dagger}] = \left(\frac{d^2}{d^2x} + \frac{d}{dx}\frac{x}{2} + \frac{x}{2}\frac{d}{dx} + \frac{x^2}{4}\right) - \left(+\frac{d^2}{d^2x} + \frac{d}{dx}\frac{x}{2} + \frac{x}{2}\frac{d}{dx} + \frac{x^2}{4}\right) = 0 , \qquad (44)$$

because all terms cancel identically. The final commutator relations are

$$[H_1, A^{\dagger}] = A^{\dagger} = [A^{\dagger}A, A^{\dagger}] = A^{\dagger}[A, A^{\dagger}] + [A^{\dagger}, A^{\dagger}]A = A^{\dagger}(1) + 0$$
(45)

$$[H_1, A] = -A = [A^{\dagger}A, A] = A^{\dagger}[A, A] + [A^{\dagger}, A]A = 0 + (-1)A , \qquad (46)$$

using the commutator identity [AB, C] = A[B, C] + [A, C]B. Therefore all commutation relations for the harmonic oscillator raising and lowering operators are satisfied by this form of W(x).

3.2 First Hamiltonian.

Now consider the Hamiltonian $H_1 = A^{\dagger}A$, assume a ground state $\psi_0(x)$ exists. Acting on this state with the lowering operator A, will give zero,

$$A |\psi_0\rangle = 0 \Rightarrow \left(\frac{d}{dx} + \frac{x}{2}\right) |\psi_0\rangle = 0 \Rightarrow \frac{d}{dx} \psi_0(x) = -\frac{x}{2} \psi_0(x) .$$

$$\tag{47}$$

For the derivative of a function to equal itself times a polynomial, solutions should be exponentials of polynomials. Since there is only a linear term in x, there must only be an x^2 term in the exponential. To get the factors of 2 to work out the ground state must be

$$\psi_0(x) = C e^{-x^2/4} , \qquad (48)$$

where C is a constant that can be determined through normalization. The normalization condition is

$$1 = \int_{-\infty}^{\infty} |\psi_0(x)|^2 dx = |C|^2 \int_{-\infty}^{\infty} e^{-x^2/2} dx = |C|^2 \sqrt{2\pi},$$
(49)

so the complete ground state wave function is

$$\psi_0(x) = \frac{1}{(2\pi)^{1/4}} e^{-x^2/4} .$$
(50)

The energy of this state can be found by acting the Hamiltonian on the state,

$$H_1 |\psi_0\rangle = E_0^{(1)} |\psi_0\rangle \implies \left(-\frac{d}{dx} + \frac{x}{2}\right) \left(\frac{d}{dx} + \frac{x}{2}\right) |\psi_0\rangle = E_0^{(1)} |\psi_0\rangle , \qquad (51)$$

the left hand side is

$$\left(-\frac{d}{dx} + \frac{x}{2}\right)\left(\frac{d}{dx}\frac{e^{-x^2/4}}{(2\pi)^{1/4}} + \frac{x}{2}\frac{e^{-x^2/4}}{(2\pi)^{1/4}}\right) = \left(-\frac{d}{dx} + \frac{x}{2}\right)\left(-\frac{x}{2}\frac{e^{-x^2/4}}{(2\pi)^{1/4}} + \frac{x}{2}\frac{e^{-x^2/4}}{(2\pi)^{1/4}}\right) = 0, \quad (52)$$

which means that $E_0^{(1)} = 0$. For higher energy eigenstates, the relationship is $H_1 |\psi_n\rangle = E_n^{(1)} |\psi_n\rangle$, but from the commutator relations, $[H_1, A] = H_1 A - A H_1 = -A$, so that

$$H_1 A |\psi_n\rangle = -A |\psi_n\rangle + A H_1 |\psi_n\rangle \Rightarrow H_1 A |\psi_n\rangle = -A |\psi_n\rangle + A(E_n^{(1)}) |\psi_n\rangle$$
(53)

$$= (E_n^{(1)} - 1)A |\psi_n\rangle , \qquad (54)$$

which corresponds to a state with a lower energy, by a value 1. The energy of the ground state is zero, and $A |\psi_1\rangle \rightarrow |\psi_0\rangle$, so $(E_n^{(1)} - 1) = 0$, or $E_n^{(1)} = 1$. Generalizing this to higher energy eigenstates, $E_n^{(1)} = n$.

The remaining eigenstates can be found by acting A^{\dagger} on the ground, and subsequent states. Acting A^{\dagger} on the ground state *n* times will result in the functional form of $\psi_n(x)$, up to a normalization factor. Consider the action of a^{\dagger} on a state $|n\rangle$ of the harmonic oscillator

$$a^{\dagger} \left| n \right\rangle = \sqrt{n+1} \left| n+1 \right\rangle \ , \tag{55}$$

and according to Shankar Equation 7.4.35, the action of a^{\dagger} , n times on the ground state is

$$(a^{\dagger})^n \left| 0 \right\rangle = \sqrt{n!} \left| n \right\rangle \ . \tag{56}$$

Therefore, with the operator A^{\dagger} , and the ground state $|\psi_0\rangle$, any eigenstate can be found using the formula

$$|\psi_n\rangle = \frac{1}{\sqrt{n!}} (a^{\dagger})^n |\psi_0\rangle \quad . \tag{57}$$

This gives the Schrödinger equation to be

$$H_1 |\psi_n\rangle = n |\psi_n\rangle, \ n = 0, 1, 2, 3...$$
 (58)

3.3 Second Hamiltonian.

This process can be repeated for a second Hamiltonian,

$$H_2 = AA^{\dagger} = 1 + H_1 , \qquad (59)$$

which can be shown through the commutator relation

$$[A, A^{\dagger}] = AA^{\dagger} - A^{\dagger}A = H_2 - H_1 = 1 .$$
(60)

To find the eigenstates of H_2 , consider the commutator

$$[H_1, H_2] = [A^{\dagger}A, AA^{\dagger}] = A^{\dagger}AAA^{\dagger} - AA^{\dagger}A^{\dagger}A , \qquad (61)$$

so from Equation 60, this becomes

$$[H_1, H_2] = A^{\dagger}A(1 + A^{\dagger}A) - (1 + A^{\dagger}A)A^{\dagger}A = A^{\dagger}A + (A^{\dagger}A)^2 - A^{\dagger}A - (A^{\dagger}A)^2 = 0 , \qquad (62)$$

and therefore H_1 and H_2 have the same eigenstates (because their commutator is zero). The eigenvalues of H_2 are related to those of H_1 by

$$H_{2} |\psi_{n}\rangle = E_{n}^{(2)} |\psi_{n}\rangle \Rightarrow (H_{1} + 1) |\psi_{n}\rangle = E_{n}^{(2)} |\psi_{n}\rangle \Rightarrow H_{1} |\psi_{n}\rangle = (E_{n}^{(2)} - 1) |\psi_{n}\rangle , \quad (63)$$

so $E_n^{(2)} = 1 + E_n^{(1)} = n + 1$. Therefore the n^{th} state of H_2 has the same energy as the $(n-1)^{th}$ state of H_1 . This gives the Schrödinger equation to be

$$H_2 |\psi_n\rangle = n + 1 |\psi_n\rangle, \ n = 0, 1, 2, 3...$$
 (64)

3.4 Action of A and A^{\dagger} .

Now would be a good time to stop and compute the action of the operators on a state $|\psi_n\rangle$. First consider the action of A, the lowering operator: $A |\psi_n\rangle = B_n |\psi_{n-1}\rangle$. To find B_n , each side can be multiplied by its complex conjugate (note that if x = y then $x^* = y^*$),

$$|B_n|^2 \langle \psi_{n-1} | \psi_{n-1} \rangle = \langle \psi_n | A^{\dagger} A | \psi_n \rangle = \langle \psi_n | H_1 | \psi_n \rangle \quad , \tag{65}$$

so that $B_n = \sqrt{n}$ by noting that the inner product of an eigenstate with itself is one. Now consider the action of A^{\dagger} , the raising operator: $A^{\dagger} |\psi_n\rangle = C_n |\psi_{n+1}\rangle$. To find C_n , each side can be multiplied by its complex conjugate,

$$|C_n|^2 \langle \psi_{n+1} | \psi_{n+1} \rangle = \langle \psi_n | A A^{\dagger} | \psi_n \rangle = \langle \psi_n | H_2 | \psi_n \rangle \quad , \tag{66}$$

so that $C_n = \sqrt{n+1}$. This gives the actions for A and A^{\dagger} :

$$A \left| \psi_n \right\rangle = \sqrt{n} \left| \psi_{n-1} \right\rangle \tag{67}$$

$$A^{\dagger} \left| \psi_n \right\rangle = \sqrt{n+1} \left| \psi_{n+1} \right\rangle \tag{68}$$

(69)

3.5 Third Hamiltonian.

Now consider the Hamiltonian

$$H = \begin{bmatrix} A^{\dagger}A & 0\\ 0 & AA^{\dagger} \end{bmatrix} = \begin{bmatrix} H_1 & 0\\ 0 & H_2 \end{bmatrix} , \qquad (70)$$

whose eigenstates can be determined from the eigenstates of H_1 and H_2 . The Schrödinger equation says

$$\hat{H}\Psi = \epsilon \Psi \implies \begin{bmatrix} H_1 & 0\\ 0 & H_2 \end{bmatrix} \begin{bmatrix} \phi\\ \varphi \end{bmatrix} = \epsilon \begin{bmatrix} \phi\\ \varphi \end{bmatrix} , \qquad (71)$$

but for the eigenstates of H_1 and H_2 to both have the same energy ϵ , they must be the eigenstates found before, but one energy level apart from each other (according to the relation in the last line of section 2.3). This makes the Schrödinger equation

$$\begin{bmatrix} H_1 & 0\\ 0 & H_2 \end{bmatrix} \begin{bmatrix} |\psi_{n+1}\rangle \\ |\psi_n\rangle \end{bmatrix} = \epsilon \begin{bmatrix} |\psi_{n+1}\rangle \\ |\psi_n\rangle \end{bmatrix} = (n+1) \begin{bmatrix} |\psi_{n+1}\rangle \\ |\psi_n\rangle \end{bmatrix} .$$
(72)

This lets the eigenstates of this Hamiltonian be defined as

$$|n\rangle = \begin{bmatrix} |\psi_{n+1}\rangle \\ |\psi_n\rangle \end{bmatrix} \quad \text{with energy} \quad \epsilon_n = n+1 .$$
(73)

3.6 *Q* **Operators.**

Consider the operators

$$Q = \begin{bmatrix} 0 & 0 \\ A & 0 \end{bmatrix} \qquad Q^{\dagger} = \begin{bmatrix} 0 & A^{\dagger} \\ 0 & 0 \end{bmatrix}$$
(74)

with [H,Q] = 0 and $[H,Q^{\dagger}] = 0$. The action of Q on the eigenstates of H is

$$Q|n\rangle = \begin{bmatrix} 0 & 0\\ A & 0 \end{bmatrix} \begin{bmatrix} |\psi_{n+1}\rangle \\ |\psi_n\rangle \end{bmatrix} = \begin{bmatrix} 0\\ A|\psi_{n+1}\rangle \end{bmatrix} = \sqrt{n+1} \begin{bmatrix} 0\\ |\psi_n\rangle \end{bmatrix} , \qquad (75)$$

and similarly for Q^{\dagger} ,

$$Q^{\dagger} |n\rangle = \begin{bmatrix} 0 & A^{\dagger} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} |\psi_{n+1}\rangle \\ |\psi_{n}\rangle \end{bmatrix} = \begin{bmatrix} A^{\dagger} |\psi_{n}\rangle \\ 0 \end{bmatrix} = \sqrt{n+1} \begin{bmatrix} |\psi_{n+1}\rangle \\ 0 \end{bmatrix} .$$
(76)

Clearly these operators do not raise or lower the $|\psi\rangle$ states in $|n\rangle$, but do destroy one of the components of $|n\rangle$. Now, consider the repeated action of Q and Q^{\dagger} on a state $|n\rangle$,

$$QQ|n\rangle = \begin{bmatrix} 0 & 0\\ A & 0 \end{bmatrix} \sqrt{n+1} \begin{bmatrix} 0\\ |\psi_n\rangle \end{bmatrix} = \sqrt{n+1} \begin{bmatrix} 0\\ 0 \end{bmatrix}$$
(77)

$$Q^{\dagger}Q|n\rangle = \begin{bmatrix} 0 & A^{\dagger}\\ 0 & 0 \end{bmatrix} \sqrt{n+1} \begin{bmatrix} 0\\ |\psi_n\rangle \end{bmatrix} = \sqrt{n+1} \begin{bmatrix} A^{\dagger} & |\psi_n\rangle \\ 0 \end{bmatrix} = (n+1) \begin{bmatrix} |\psi_{n+1}\rangle \\ 0 \end{bmatrix}$$
(78)

$$QQ^{\dagger}|n\rangle = \begin{bmatrix} 0 & 0\\ A & 0 \end{bmatrix} \sqrt{n+1} \begin{bmatrix} |\psi_{n+1}\rangle \\ 0 \end{bmatrix} = \sqrt{n+1} \begin{bmatrix} 0\\ A |\psi_{n+1}\rangle \end{bmatrix} = (n+1) \begin{bmatrix} 0\\ |\psi_n\rangle \end{bmatrix}$$
(79)

$$Q^{\dagger}Q^{\dagger}|n\rangle = \begin{bmatrix} 0 & A^{\dagger} \\ 0 & 0 \end{bmatrix} \sqrt{n+1} \begin{bmatrix} |\psi_{n+1}\rangle \\ 0 \end{bmatrix} = \sqrt{n+1} \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
(80)

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From this, repeated action of the same operator on a state $|n\rangle$ destroys the state and results in zero. However, alternating actions of Q and Q^{\dagger} flips the state of the previous action and adds a factor of $\sqrt{n+1}$. Therefore no matter how many alternating actions of either operator are performed on a state $|n\rangle$, the only states that can result are

$$\begin{bmatrix} 0\\ |\psi_n\rangle \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} |\psi_{n+1}\rangle\\ 0 \end{bmatrix} \tag{81}$$

times a factor of $(n + 1)^{k/2}$, where k is an integer that denotes how many times the alternating actions of Q and Q^{\dagger} were performed. The matrix elements of Q can be calculated:

$$\langle m|Q|n\rangle = (\langle \psi_{m+1}|\langle \psi_m|) \begin{bmatrix} 0 & 0\\ A & 0 \end{bmatrix} \begin{bmatrix} |\psi_{n+1}\rangle\\ |\psi_n\rangle \end{bmatrix} = (\langle \psi_{m+1}|\langle \psi_m|)\sqrt{n+1} \begin{bmatrix} 0\\ |\psi_n\rangle \end{bmatrix}$$
(82)

$$=\sqrt{n+1}\left\langle\psi_{m}|\psi_{n}\right\rangle=\sqrt{n+1}\delta_{mn},\qquad(83)$$

where δ_{mn} is the Kronecker delta function. This implies that Q is a diagonal matrix in the basis for which H is diagonal. Similarly, for Q^{\dagger} :

$$\langle m|Q^{\dagger}|n\rangle = \left(\langle\psi_{m+1}|\langle\psi_{m}|\right) \begin{bmatrix} 0 & A^{\dagger} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} |\psi_{n+1}\rangle \\ |\psi_{n}\rangle \end{bmatrix} = \left(\langle\psi_{m+1}|\langle\psi_{m}|\rangle\sqrt{n+1} \begin{bmatrix} |\psi_{n+1}\rangle \\ 0 \end{bmatrix}$$
(84)

$$=\sqrt{n+1}\langle\psi_{m+1}|\psi_{n+1}\rangle = \sqrt{n+1}\delta_{mn} \ . \tag{85}$$

The matrix elements of Q and Q^{\dagger} were calculated for the $\{|n\rangle\}$ basis (eigenbasis of H) and are only nonzero for matrix indeces m = n. Therefore in this basis, both matrices are diagonal, so the eigenvalues of these matrices are the values of the diagonal entries. The eigenvalues are then $\sqrt{n+1}$ for $n = 0, 1, 2, 3, \ldots$

Additionally, it can be noted the sum of these operators is

$$(Q+Q^{\dagger})|n\rangle = \begin{bmatrix} 0 & A^{\dagger} \\ A & 0 \end{bmatrix} \begin{bmatrix} |\psi_{n+1}\rangle \\ |\psi_n\rangle \end{bmatrix} = \sqrt{n+1} \begin{bmatrix} |\psi_{n+1}\rangle \\ |\psi_n\rangle \end{bmatrix} , \qquad (86)$$

and taking the square of the sum,

$$(Q+Q^{\dagger})^2 = \begin{bmatrix} 0 & A^{\dagger} \\ A & 0 \end{bmatrix} \begin{bmatrix} 0 & A^{\dagger} \\ A & 0 \end{bmatrix} = \begin{bmatrix} A^{\dagger}A & 0 \\ 0 & AA^{\dagger} \end{bmatrix} = H .$$
(87)