Entanglement in Quantum Harmonic Chains

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Abstract

Harmonic chains are used as a model in quantum information theory for ion traps and simple solid state systems. Entanglement is a quantum effect in which observations made on one object instantaneously affect measurement outcomes on the other. This study investigates interparticle entanglement in finite chains of coupled harmonic oscillators as a function of the vibrational modes, mode excitations, and bipartition of oscillators. The methods used and results extend previous work for the Gaussian ground state to excited states. Entanglement is analyzed by calculating the purity of the reduced density matrix of the combined wavefunctions of the oscillators in the chain, tracing over subensembles. Analytic and numerical results for a varying effective spring constants between the particles and number of particles in the chain are presented. Interesting correlations between the symmetries of the vibrational modes and their excitations, and the symmetries of the partitions were discovered. Results show that higher excitation numbers result in higher entanglement. Adding energy to the modes will never decrease entanglement, however, the relationship between energy and entanglement is not simple. Different combinations of mode energy excitations will produce the same entanglement, even if the total energy of the system differs. Patterns indicate that the combination of symmetry in mode shapes and partition determines excitation number purity equivalence classes.

1 Introduction

1.1 Setup

In this study we investigate entanglement in finite quantum harmonic chains: coupled quantum harmonic oscillators in 1D, bound by fixed edges (see Figure 5). We observe how the vibrational modes, mode excitation number / energy eigenstates, and symmetries of the bipartitions of oscillators affects the entanglement of the system.

1.2 Motivation, Applications of Entanglement

As our technology allows us to more precisely manipulate individual atoms and particles, we inch closer towards being able to build quantum computers which will exponentially increase the computational power of computing machines and processors. Instead of using transistors as the unit of processing, which can only carry current in binary signals ("on" or "off"), quantum systems will exponentially increase computational power as their processors can be $|0\rangle$ and $|1\rangle$ at the same time, as well as an infinite amount combinations (superpositions) of the two (like $1/\sqrt{2}|0\rangle 1/\sqrt{2}|1\rangle$). Obtaining the knowledge to fully understand, quantify, and manipulate entanglement in quantum systems is a crucial step towards achieving this technology.

Entanglement is also involved in phase transitions, and has implications in superconductivity, the basis of which are entangled pairs of electrons in a metal. Additionally, it has recently been discovered that the photosynthesis complex in plants absorbs photons in entangled pairs and use entanglement to efficiently transport that energy [1]. Understanding this phenomena could allow the development of vastly more efficient solar cell technology. Harmonic chains are also of interest as they are used as a model in quantum information theory for ion traps, simple solid state systems, and lattices.

1.3 Background

Previously, properties of harmonic oscillators have been studied, though most work has only focused on the ground state and not the excited states [2]. Density matrix theory applied to entangled systems have been extensively analyzed and described [3][4]. Specifically it has been applied to one example of the 2-body quantum harmonic chain, massive coupled oscillators, and has been used to examine properties of excited states. The calculation methods used in this study build off gaussian wave function analysis explained by Harshman [4] and the density matrix methods used by Harshman and Flynn [5].

1.4 Methods

We model quantum harmonic chains using the classical model of coupled oscillators (see Figure 5). We calculate the relative normal mode frequencies, and the relative amplitudes of each particle in each mode. Using the general equation for the quantum harmonic oscillator, we use a coordinate transformation from configuration space into position space to produce a function that includes the positions of the particles for each mode. We then take the product of the wavefunctions of each mode, since any configurations of particles are a superposition of the vibrational modes. We measure entanglement by calculating the purity of the reduced density matrix, tracing over subensembles and discarding the appropriate irrelevant interparticle correlations.

1.5 Summary of Results

Our results show that generally higher mode excitation numbers result in higher entanglement. Exciting modes will never decrease entanglement, however the relationship between energy and modes is not that simple. For example, in the 1v23 partition of the 3-body system, mode excitation indices of $\{2,0,1\}$ and $\{1,0,2\}$ are equally entangled, even though the latter system has more energy. We have discovered that the combination of symmetry of mode shapes and partition determines the excitation number purity equivalence classes. We are in the process of analyzing the 4-body system and are searching for more patterns, which we think will find the most generalizable form for our results.

2 Entanglement

As mankind's understanding of the universe and technology advances, we are now observing and experimenting with matter on the smallest scales. In the regime of the infinitesimally small, a different set of rules dictates physics: quantum mechanics. Quantum mechanics provides for many phenomena that seem quite bizarre by our classical conception of the universe, one of the most notorious being quantum entanglement.

Entanglement is a quantum effect in which observations made on one object instantaneously affect measurement outcomes on the other. It is essentially a measure of non-classical correlation between two objects or groups of objects (called partitions). If two objects are entangled, measurements on one object will instantaneously affect measurements made on the other it is entangled with, regardless of the distance separating them. In the words of Albert Einstein, it is like "spooky action at a distance". One author provides a helpful explanation of entanglement:

"For quantum particles to be entangled, they must both have been part of the same larger system/object at one time. When the larger object to which they both belonged no longer holds its integrity, its parts are no longer physically yoked. These now freed quantum particles may relocate to entirely different places in the universe, but they never forget their original family, so what happens to their previous family members continues to affect them." [6]

2.1 Particle Analogy

For example, let's say a particle with 0 spin decays into two other particles. Conservation laws hold that the sum of the spin of the system after the decay must still be 0. So one particle might have a spin of +1, and the other -1. Now hypothetically, two experimenters, Alice and Bob, each take one particle from the entangled pair and separate. When Alice goes to measure the spin of her particle, her results will be totally unpredictable: she has a 50% chance of measuring a spin of +1, and a 50% chance of measuring a spin of -1. Alice measures her spin as +1. If Bob now measures his, the measurement is predictable: it will always be the opposite of what Alice measured. Alice's measurement affected the measurement Bob will make. If Alice then measures a -1, Bob will observe a +1 spin on his particle. This analogy is example of correlation, not quite entanglement.

There is often speculation as to the implications of entanglement in faster-than-light communication. Unfortunately, entanglement can not be used to break the universal speed limit. For example, if Bob measures his particle and gets a value of -1, he does not know if he observed a -1as a result of randomness or if it is because Alice measured her entangled particle as +1, and won't know until he communicates with her. The communication between Alice and Bob can not occur faster than the speed of light.

2.2 Quantifying Entanglement

Considering the previous analogy, one might ask "how entanglement can be quantified", or "isn't it a binary 'yes' or 'no' quality"? The answer to that is no. Let's say now instead of a binary particle system, Alice and Bob now have a set of magic dice. In one scenario, if Alice rolls a 1, then Bob will roll a 1, 3, or 5. Alice's roll will affect Bob's roll, but it does not directly dictate his exact outcome. There is still some uncertainty and randomness in Bob's outcome, but Bob's outcome is correlated with Alice's, so in this case the "entanglement" of the dice can be quantified by some fraction. But again, if Bob rolls a 3, he has no way of knowing if he rolled a 3 because Alice rolled a 1, or because he randomly happened to roll a 3, until Alice tells him she made a measurement, or "rolled the die".

2.3 Correlation & Entanglement

There is a difference between entanglement and correlation, and it is oft most effectively described at first using another analogy. Let's say Alice and Bob are exploring and wish to know the topography of the land. They split up; Alice is on the west side of an area, and Bob is on the south side of an area. It is dusk, so they can only see the silhouettes of the topography. Alice looks east and sees the shape in Figure 1 (left), two "mountains", and Bob looks north and sees the "mountain" in Figure 1 (right).

"The motion of a single particle depends on the positions of the other particles, rather than on some average density. Consequently, in a system of interacting particles, the probability of finding



Figure 1: The left figure represents Alice's view, looking east. The right figure depicts Bob's view, looking north.

two particles with given positions or momenta is not simply the product of the single-particle probabilities: We say that the particles are 'correlated''.[3]

When they combine their data, or observations, the topography of the land becomes clear: "two mountains" (a northern one and a southern one), as shown in Figure 2.

Now imagine if Alice and Bob saw the silhouettes in Figure 3 (left), instead of the ones in Figure 1. If they combined their data, it would indicate that the mountain would look like the depiction in Figure 3 (right).

However, if the system they were observing was entangled, they would not be getting the complete picture here. To determine what they are really seeing, they would have to make a series of *measurements* and then *correlate* their measurement data with each other. For example, let's say that Alice and Bob both see a series of different color lightning bolts hit the top of the mountain. If they just simply combined their data, they would have observed the lightning hitting the top in a guassian shape, and concluded the shape was that shown in Figure 3 (right). Now, if Alice and Bob compare their data, they will now that Alice say the red lightning bolt hit in the south, and that Bob saw that same bolt hit in the east, meaning it hit in the southeast. Alice saw the pink bolt hit in the north, and Bob saw the pink bolt hit in the west, indicating the mountain's top at that position is northwest. Correlating the rest of their data, they will see that the mountain takes the shape of a gaussian, but that it is squeezed/slanted, as shown in Figure 5.

This is an example of an entangled system. An entangled system can not be fully described without knowing the *correlation* between two sets of data. This mountain example is an analogy for entanglement diagrams, where the projection of the mountain onto one of the axes (Alice's or Bob's "view") is the probability distribution (measurements) of one particle of the two particles or groups. So to completely describe an entangled system of particles, one needs to know the correlation between the measurements of the first particle and the measurements on the second



Figure 2: Combination of Alice's and Bob's data gives the complete description of the land



Figure 3: Top left: Alice's view. Bottom left: Bob's view. Right: assumed combination of their views



Figure 4: Top left: Alice's view. Bottom left: Bob's view. Right: assumed combination of their views

particle.

3 Model & Methods

We use the classical model of coupled oscillators (masses linked by springs), to model harmonic chains, as the same equations for mode frequencies, relative amplitudes of the modes, and normal mode shapes describe their behavior. Any pattern of motion of the masses can be described as a combination of the excitations (or "multiples") of the system's vibrational modes. One can think of modes as the smallest units of vibrational motion of which comprise and describe the entire system's internal motion. Mode excitations numbers are non-negative integers.

Figure 5 depicts the normal mode shapes for each of the three systems investigated. For the 2-body system, there are 2 modes: one symmetric mode in which the masses oscillate in the same direction with the same amplitude, and an antisymmetric mode in which the masses oscillate opposite in directions also with the same amplitude. For the 3-body system, there are 3 modes: mode 1 in which the masses oscillate in the same direction but with varying amplitudes, mode 2 in which the middle mass is stationary while the other two oscillate antisymmetrically, and mode 3 in which masses 1 and 3 oscillate in the same direction, while mass 2 oscillates in the opposite. For the 4-body system there are 4 modes, following the same pattern.



Figure 5: Top: 2-body system. Middle: 3-body system. Bottom: 4-body system. Curved lines depict the normal mode shapes. Positive amplitude of the curve means the particle vertically aligned with that point is moving to the right of its initial position, negative amplitude corresponds with moving to the left, as illustrated by the red and blue arrows in the top box

3.1 Mode Frequency

We use the general equation for mode frequency

$$\omega_{\nu} = 2\sqrt{\frac{k}{m}} \sin\left[\frac{\pi\nu}{2(N+1)}\right] \tag{1}$$

where ω_{ν} is the frequency of mode ν , k is the effective spring constant between the particles, m is mass, and N is the number of the masses. There are N modes for a chain with N masses. [7]

3.2 Relative Mode Amplitudes

We also use the general equation for the relative amplitudes of the particles in each mode

$$a_{j,\nu} = \sqrt{\frac{2}{N+1}} \sin\left[\frac{\pi j\nu}{N+1}\right] \tag{2}$$

where j represents the jth mass in the chain for mode ν . [7] For example, $a_{3,2}$ represents the relative amplitude of the 3rd particle in the 2nd mode. The amplitudes of a system can be represented by a matrix, such as the one in Figure 6. These matrices can be used as a transformation from configuration space (which describes the system in terms of the modes) to position space (which describes the system more explicitly in terms of the amplitudes of the particles, or their positions).

Relative Amp of particle

$$\mathbf{M} \left(\begin{array}{ccc} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{array} \right)$$

Figure 6: Matrix for the 3-body system. Rows represent the modes, and the 1st, 2nd, and 3rd entries in each mode represent the relative amplitudes of the 1st, 2nd, and 3rd particle, respectively

3.3 Quantum Harmonic Chains

We describe each system using the product of the wave functions of quantum harmonic oscillators.

$$\psi_{\nu,n}(\mathbf{x}) = \left[\frac{m\omega_{\nu}}{\pi\hbar}\right]^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi_{\nu}(\mathbf{x})) \exp\left[-\frac{m\omega_{\nu}}{2\hbar} \left\{\xi_{\nu}(\mathbf{x})\right\}^2\right]$$
(3)

where $\psi_{\nu,n}$ is the wave function for the *n*th excitation of mode ν , H_n is the Hermite polynomial for ξ_{ν} .

$$\xi_{\nu}(\mathbf{x}) = \sqrt{\frac{m\omega_{\nu}}{\hbar}} \left[\sum_{j=1}^{N} a_{j,\nu} x_j \right]$$
(4)

and x_j is the position of mass j. ξ_{ν} represents the configuration of particles x_1 through x_j , each weighted by its respective relative amplitude for mode ν , normalized by the length scale of the mode, which is scaled to a dimensionless quantity.

The **x** vector

$$\mathbf{x} = \{x_1, x_2, \dots, x_N\}\tag{5}$$

represents the particles 1 through N.

3.4 Energy of the Quantum Harmonic Chain

The energy scale of a quantum harmonic oscillator is given by the equation

$$E = \hbar \omega \left\{ n + \frac{1}{2} \right\} \tag{6}$$

where n is the excitation number. The energy of a quantum harmonic chain can be given by the sum of the energies of the modes, given by

$$E = \hbar \sum_{\nu=1}^{N} \omega_{\nu} \left\{ n_{\nu} + \frac{1}{2} \right\}$$
(7)

where n_{ν} is the excitation number for mode ν , and ω_{ν} is the frequency of mode ν .

From Eq. 1, higher modes have higher frequencies, so exciting higher modes requires more energy than exciting lower modes. For example, for the 2-body system, $\omega_1 = \sqrt{\frac{k}{m}} = \omega_0$ and $\omega_2 = \sqrt{3}\omega_0$. For the 3-body system, $\omega_1 \approx .765\omega_0$, $\omega_1 \approx 1.41\omega_0$, and $\omega_3 \approx 1.85\omega_0$.

4 Purity

4.1 Calculating Purity

In all of the above equations, \hbar , k, and m were set to equal 1 to use natural units for this system. To analyze entanglement, we calculate the purity of the reduced density matrix of the combined wave functions, tracing over subensembles. This was accomplished using Mathematica's numerical integration function. For systems in the ground state, we can also calculate the exact results using matrices. The purity represents the entanglement of the system on a scale of 0 to 1, 0 meaning maximal entanglement, and 1 meaning no entanglement. Alternatively, another way of representing entanglement is the Schmidt number, which is simply 1 divided by the purity, or just the inverse of the purity. The Schmidt number is advantageous in certain systems to produce a larger spread of values, for ease of comparison.

The wave function

$$\Psi_{\{n_i\}}(\mathbf{x}) = \prod_{i=1}^{N} \psi_{\nu_i, n_i}(\mathbf{x})$$
(8)

is the product of wave functions $\psi_{\nu,n}$ for each mode ν at the *n*th excitation. The sigma vector represents the particles of one partition, primed. In this case, for the 3-body example, the partition of particles 1 & 3 vs 2 is

$$\sigma_{\mathbf{p}}(\mathbf{x}, \mathbf{x}') = \{x_1, x_2', x_3\}\tag{9}$$

The σ prime vector represents the particles of the other partition, primed.

$$\sigma_{\mathbf{p}}'(\mathbf{x}, \mathbf{x}') = (x_1', x_2, x_3') \tag{10}$$

The purity is the integral of the product of wave functions $\Psi_{\nu,j}(\vec{x})$ for the primed and unprimed x and σ vectors.

$$P(N, \{\nu_i\}, p) = \int d^N \vec{x} \, d^N \vec{x}' \, \Psi_{\{\nu_i\}}(\vec{x}) \, \Psi_{\{\nu_i\}}(\vec{x}') \, \Psi_{\{\nu_i\}}(\vec{\sigma_p}) \, \Psi_{\{\nu_i\}}(\vec{\sigma_p}') \tag{11}$$

The set $\{\nu_i\}$ represents the set of mode excitation indices. The 1st entry represents the excitation of the 1st mode, and the Nth entry represents the excitation of the Nth mode. For example, (2,0,1)means that the 1st mode is in the 2nd excited state, the 2nd mode is in the ground state, and the 3rd mode is in the 1st excited state.

4.2 Error Analysis & Cross Checking

The purity integral (Eq. 11) was evaluated using the numerical integrate function in Mathematica. Excited state integrals could not be evaluated from $\pm \infty$ efficiently because of limitations in computational power and integration algorithms, so the limits of integration were usually set to ± 3 . Error analysis showed that the integrals of the excluded range ($-\infty$ to -3, or 3 to $+\infty$) are on the order of 10^{-17} to 10^{-22} , so we can conclude that the modified limits of integration have a negligible effect on our results. For example, for the $\{1, 1, 1\}$ excited state of the 3-body system, the value for the purity integral integrated from $-\infty$ to -2 was $8.04 * 10^{-17}$, a negligible amount.

We cross-checked our numerical results by comparing them to exact results obtained using the coherent state method from Reference [3]. Our results for the 2- and 3-body were accurate to 1 part in 10,000. Our numerical results were both sometimes slightly over and slightly under the exact results, which indicates that discrepancies resulted from random error, and not systematic error, as negligible as they were. Our results for the 4-body were accurate to 1 part within 1,000.

5 Results

5.1 2-Body System: 2 Particles, 1 Spring Constant

Our results show that increasing mode excitation increases entanglement, but that switching the mode excitation numbers does not change the entanglement. For example, exciting the 1st mode to $\nu_1 = 3$ and the 2nd mode to $\nu_2 = 1$ is equally entangled as a system with $\nu_1 = 1$ and $\nu_2 = 3$.

This is summarized by the equation

$$1v2 \to (\boldsymbol{a}, \boldsymbol{b}) = (\boldsymbol{b}, \boldsymbol{a}) \tag{12}$$

The hypothesized explanation for this is that in both modes the correlation between the particles is the same: they are either symmetric or antisymmetric, so switching the weights of the amplitudes of symmetric and antisymmetric oscillation patterns does not change their correlation.

5.2 2-Body System: 2 Particles, 2 Spring Constants (Ground State)

This system differs slightly in that the middle spring constant connecting particles 1 and 2 is of a different value from the outer spring constants. A graphical representation of this system is given in Figure 7.

For equal masses and an unequal middle spring, we derived an equation for purity as a function of the different spring constants (or mode frequencies). We applied the substitutions given by equations 14 - 16 analytically in Mathematica into the equation for purity (Eq. 11). Purity is given by

$$P = \frac{2\sqrt{\delta}}{1+\delta} \tag{13}$$



Figure 7: Left: Entanglement as a function of mode excitation number. Values of the same color represent equivalence. Slight discrepancies between equivalent values are the result of random integration error. $i_{\omega}1$ represents the *i*th excitation of mode ω_1 , $i_{\omega}2$ represent the *i*th excitation of mode ω_2 . Right: 3D graph of the data from the left. Entanglement approximately doubles as a mode enters the 1st excited state, and continues to increase as mode excitation increases



Figure 8: Graphical representation of the 2-body system with unequal spring constants



Figure 9: Plot of purity as a function of δ . Purity asymptotically approaches 0 as δ approaches infinity.

where

$$\delta = \frac{\omega_2}{\omega_1} \tag{14}$$

$$\omega_1 = \sqrt{\frac{k_1}{m}} \tag{15}$$

and

$$\omega_2 = \sqrt{\frac{k_1 + 2k_2}{m}} \tag{16}$$

For the ground state, as k_2 becomes increasingly high, the system becomes increasingly entangled, as shown in Figure 8.

5.3 3-Body System

For the 13v2 partition, the excitation indices for the 1st and 3rd mode can be switched and the purity will be kept the same, regardless of how much the 2nd mode is excited or changed.

$$13v2 \to (\boldsymbol{a}, \boldsymbol{c}, \boldsymbol{b}) = (\boldsymbol{b}, \boldsymbol{d}, \boldsymbol{a}) \tag{17}$$

For the 1v23 partition, the 1st and 3rd mode indices can be switched and the purity will remain the same, as long as the excitation index for the 2nd mode is kept constant.

$$1v23 \to (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) = (\boldsymbol{c}, \boldsymbol{b}, \boldsymbol{a}) \tag{18}$$

Some 13v2 purity equivalence classes include:

- $(0,0,0) = (0,1,0) = (0,2,0) \approx .910$
- $(1,0,0) = (0,0,1) = (1,1,0) = (0,1,1) = (1,2,0) = (0,2,1) \approx .494$
- (2,0,0) = (0,0,2) = (2,1,0) = (0,1,2) = .364

Some 1v23 purity equivalence classes include:

- $(1,0,0) = (0,0,1) \approx .595$
- $(2,0,0) = (0,0,2) \approx .446$
- $(1,1,0) = (0,1,1) \approx .370$
- $(2,0,1) = (1,0,2) \approx .341$

Assuming no accidental degeneracies, if the values for the states were within 1 part in 1,000 of each other, we concluded that the states had equivalent purity values. In the 2-body error analysis, two results that differed by less than 1 part in 1,000 actually had the same exact analytical value, meaning that the small discrepancies were the result of random error and not accidental degeneracies. Extrapolating from that trend, we concluded that very close results represented states of equivalent purity.

For the 13v2 partition, exciting the 2nd mode affects particles 1 & 3 symmetrically, but has no effect on 2 as its amplitude is always 0, so the correlation between 1 & 3 vs 2 isnt changed. It's always $\{Amp, 0, -Amp\}$.

For the 1 v 23, exciting the 2nd mode changes the correlation (or difference) between particles 2 and 3 (by changing 3 and not 2), so the correlation between 1 vs 2 & 3 is changed.

5.4 4-Body System

We are currently still in the process of computing entanglement values for the 4-body system. Some equivalence classes are evident, though more data is needed to be certain of their patterns. The equations for them are purely hypothetical.

Some 14v23 purity equivalence classes include:

- $(1,0,0,0) = (0,1,0,0) = (0,0,1,0) \approx 1.872$
- $(1,0,0,1) = (0,1,0,1) = (0,0,1,1) \approx 5.02$
- $(0,1,1,1) = (1,0,1,1) = (1,1,0,1) \approx 8$

- $(a, b, b, c) = (b, a, b, c) = (b, b, a, c), a \neq b$, and $\{b = c \text{ or } a = c\}$
- $(1,1,0,0) = (0,1,1,0) = (0,0,0,1) \approx 3.03$

Some 14v23 purity equivalence classes include:

- $(1,0,0,0) = (0,1,0,0) = (0,0,1,0) \approx 2.13$
- $(0,1,1,1) = (1,0,1,1) = (1,1,0,1) \approx 8.55$
- $(0,1,1,1) = (1,0,1,1) = (1,1,0,1) \approx 8$
- $(a, b, b, b) = (b, a, b, b) = (b, b, a, b), a \neq b$

Some 14v23 purity equivalence classes include:

- $(1,0,1,0) = (0,1,1,0) = (0,0,1,1) \approx 4.54$
- (a, b, A, b) = (b, a, A, b) = (b, b, A, a)

Some 1v234 purity equivalence classes include:

- $(0, 1, 0, 0) = (0, 0, 1, 0) \approx 1.96$
- $(0, 1, 0, 1) = (0, 0, 1, 1) \approx 3.70$
- (a, a, a, c) = (a, a, b, c)?
- (a, b, c, d) = (a, c, b, d)?

5.5 Conclusion

Our results show that there are evident yet not fully understood patterns of mode symmetries, partition symmetries, and mode excitations that affect the entanglements of a system and determine purity equivalence classes. We believe that as we collect more results for the 4-body system, these patterns might become clearer and that we might be able to fully describe these trends with a generalizable formula or relationship. Our next step in better understanding these trends is to further analyze the mathematical properties and symmetries of the purity equation for the excited states, and in doing so develop a theoretical justification for our results.

6 References

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