DEPARTMENT OF PHYSICS

Supervised Learning Project

Effects of zero modes on quantum entanglement

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1 Introduction

Quantum entanglement ([1], [2]) is a physical phenomenon that occurs when a group of particles are generated, interact, or share spatial proximity in a way such that the quantum state of each particle of the group cannot be described independently of the state of the others. There are various measures to quantify entanglement. This is a study of entanglement present in a coupled harmonic oscillator system following the Von Neumann definition of entanglement entropy derived from the field of information theory. We study the contribution of zero modes to the divergence of the entanglement entropy of the system for the cases of positive and negative coupling constants. The results are presented using the coordinate space and Fock space formalism. We also calculate the entanglement energy following the definition from [3].

1.1 Entanglement Entropy

Consider two particles labeled A and B. The Hilbert space for the individual particles is labeled as H_A and H_B respectively and spanned by vectors $\{|a_1\rangle, |a_2\rangle, ...\}$ and $\{|b_1\rangle, |b_2\rangle, ...\}$ respectively. The Hilbert space of the system of the two particles is given by $H_A \otimes H_B$ spanned by $\{|a_i\rangle \otimes |b_j\rangle \otimes \forall |a_i\rangle, |b_j\rangle\}$.
Therefore the two particle wavefunction $|\Psi\rangle_{AB}$ can be written as:

$$|\Psi\rangle_{AB} = \sum_{ij} C_{ij} |a_i\rangle \otimes |b_j\rangle \tag{1}$$

Since the wavefunction of a system completely describes it, from the definition of entanglement entropy we can say that if we cannot write the wavefunction of the particle A independently of the wavefunction of particle B (i.e. direct product o individual waveunctions), then the particles are entangled. Mathematically it can be stated as follows:

$$|\Psi\rangle_{AB} \neq |\Psi\rangle_A \otimes |\Psi\rangle_B \tag{2}$$

for any $|\Psi\rangle_A$ in H_A and$|\Psi\rangle_B$ in H_B. To quantify the entanglement entropy we look at the density matrix for the system.
The density matrix is given by:

$$\hat{\rho}_{AB} = |\Psi\rangle\langle\Psi| \tag{3}$$

This is useful in studying the properties of the individual particles, given the wavefunction. If a subsystem A is (possibly) entangled with some other subsystem B, the information required to calculate all partial measurement outcomes on A is stored within a reduced density matrix $\hat{\rho}_A$ defined as the partial trace of $\hat{\rho}_{AB}$ over the Hilbert space of particle B, i.e.

$$\hat{\rho}_A = Tr_B(\hat{\rho}_{AB}) \tag{4}$$

Now we define the Von Neumann Entanglement Entropy of the particle A as:

$$S_A = -Tr(\hat{\rho}_A \ln \hat{\rho}_A) \tag{5}$$

$$S_A = -\sum_{n=1}^{\infty} p_n \ln p_n \tag{6}$$

where p_n are the eigenvalues of the reduced density matrix $\hat{\rho}_A$. This definition derives from the entropy concept of classical thermodynamics and information theory. These ideas are applied on a coupled harmonic oscillator system with positive and negative coupling constants. The study is performed in the coordinate space basis and the Fock space basis and there implications are discussed in the following sections.

1.2 Two Coupled Harmonic Oscillators

Consider the coupled harmonic oscillator system defined by the Hamiltonian:

$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + \frac{1}{2}m\omega^2(\hat{x}_1^2 + \hat{x}_2^2) + \frac{\alpha}{2}(\hat{x}_1 - \hat{x}_2)^2 \tag{7}$$

, α can be positive or negative. $\alpha = 0$ corresponds to two free harmonic oscillators. To analytically solve for the wavefunction of the system, we perform a coordinate transformation $\hat{x}_\pm = (\hat{x}_1 \pm \hat{x}_2)/\sqrt{2}$ and $\hat{p}_\pm = (\hat{p}_1 \pm \hat{p}_2)/\sqrt{2}$. Under this transformation the Hamiltonian becomes:

$$\hat{H} = \frac{\hat{p}_+^2}{2m} + \frac{\hat{p}_-^2}{2m} + \frac{1}{2}m\omega_+^2\hat{x}_+^2 + \frac{1}{2}m\omega_-^2\hat{x}_-^2 \tag{8}$$

where

$$\omega_+ = \omega;\ \omega_- = \sqrt{\omega^2 + \frac{2\alpha}{m}} \tag{9}$$

This Hamiltonian corresponds to a system of two uncoupled harmonic oscillators in the $x_\pm$ basis and is easier to work with analytically.

2 Entanglement Entropy Calculations in Coordinate space

The ground state of the Hamiltonian (Eq(8)) is considered and its entanglement entropy calcultions peromed. The ground state wavefunction for a harmonic oscillator is given by[4]:

$$\Psi_0(x) = \left(\frac{\beta}{\pi}\right)^{\frac{1}{4}} e^{-\beta x^2} \tag{10}$$

$\beta = \frac{m\omega}{\hbar}$
Therefore the ground state wavefunction for the given Hamiltonian (Eq(8)) is:

$$\Psi_0(x_+,\ x_-) = \frac{(\beta_+\beta_-)^{\frac{1}{4}}}{\sqrt{\pi}} e^{-\beta_+ x_+^2 - \beta_- x_-^2} \tag{11}$$

In the coordinate basis, the wavefunction is given by:

$$\Psi_0(x_1,\ x_2) = \frac{(\beta_+\beta_-)^{\frac{1}{4}}}{\sqrt{\pi}} \exp\left\{-\frac{\beta_+(x_1 + x_2)^2}{4} - \frac{\beta_-(x_1 - x_2)^2}{4}\right\} \tag{12}$$

The density matrix ($\rho_0 = |\Psi\rangle\langle\Psi|$) for this system is given by:

$$\rho_0(x_1,\ x_2,\ x_1',\ x_2') = \Psi_0(x_1,\ x_2)\Psi_0(x_1',\ x_2') \tag{13}$$

Based on Eq(4) we calculate the partial trace of ρ_0 as:

$$\rho_0(x_1,\ x_1') = \int_{-\infty}^{\infty} \Psi_0(x_1,\ x_2)\Psi_0(x_1',\ x_2')dx \tag{14}$$

$$\rho_0(x_1,\ x_1') = \int_{-\infty}^{\infty} \frac{(\beta_+\beta_-)^{\frac{1}{2}}}{\pi} \exp\left\{-\frac{\beta_+(x_1+x_2)^2}{4} - \frac{\beta_-(x_1-x_2)^2}{4} - \frac{\beta_+(x_1'+x_2')^2}{4} - \frac{\beta_-(x_1'-x_2')^2}{4}\right\} dx \tag{15}$$

$$\rho_0(x_1,\ x_1') = \frac{(\beta_+\beta_-)^{\frac{1}{2}}}{\pi} \times \frac{\sqrt{2\pi}}{(\beta_+ + \beta_-)} \times \exp\left[-\frac{1}{4}\left\{(\beta_+ + \beta_-)(x_1^2 + x_1'^2) - \left(\frac{\beta_+ - \beta_-}{\beta_+ + \beta_-}\right)^2 \frac{(x_1 + x_1')^2}{2}\right\}\right] \tag{16}$$

$$\rho_0(x_1,\ x_1') = \sqrt{\frac{\gamma_1 - \gamma_2}{\pi}} \times \exp\left\{-\frac{\gamma_1(x_1^2 + x_1'^2)}{2} - \gamma_2 x_1 x_1'\right\} \tag{17}$$

where

$$\gamma_1 = \frac{\beta_+^2 + \beta_-^2 + 6\beta_+\beta_-}{4(\beta_+ + \beta_-)},\ \gamma_2 = \frac{(\beta_+ - \beta_-)^2}{4(\beta_+ + \beta_-)}$$

To find the eigenvalues (Eq(6)), we need to solve the following equation for p_n:

$$\int_{-\infty}^{\infty} \rho_0(x_1,\ x_1') f_n(x_1') dx_1' = p_n f_n(x_1) \tag{18}$$

The solution is given by:

$$p_n = (1-\xi)\xi^n \tag{19}$$

$$f_n(x) = H_n(\sqrt{\sigma}x)\exp\{-\sigma\frac{x^2}{2}\} \tag{20}$$

where,

$$\sigma = \sqrt{\beta_+\beta_-},\ \xi = \frac{\gamma_2}{\gamma_1 + \sigma} = \left\{\frac{\sqrt{\omega_-} - \sqrt{\omega_+}}{\sqrt{\omega_-} + \sqrt{\omega_+}}\right\}^2$$

Therefore, the Neumann entropy is given by:

$$S(\xi) = -\sum_{n=1}^{\infty} p_n(\xi)\ln p_n(\xi)$$

$$S(\xi) = -\ln(1-\xi) - \frac{\xi}{1-\xi}\ln\xi \tag{21}$$

To understand the significance of normal modes in the form of entanglement entropy, we need to look at the form of ξ.

From Eq(21), entanglement entropy diverges for $\xi \to 1$ (Fig. 1).

Two cases arise:

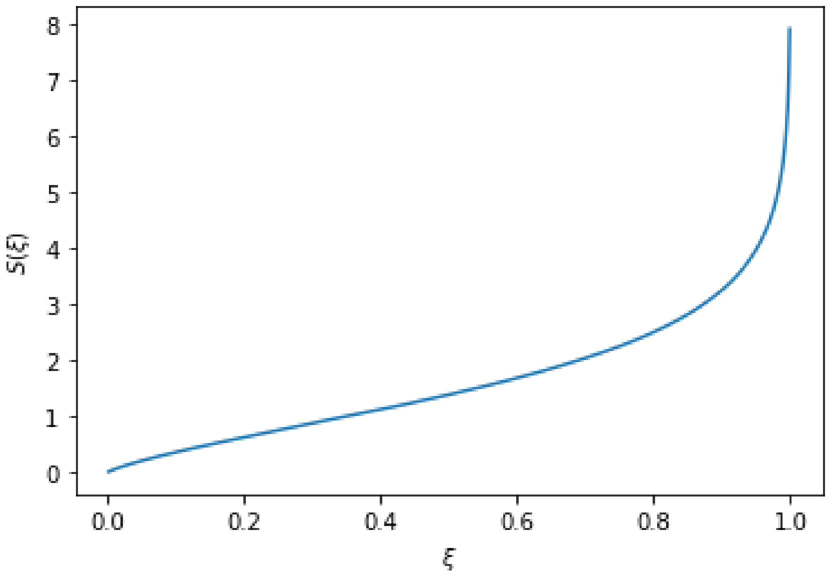


Figure 1: Entanglement energy for a coupled harmonic oscillator. $\xi \to 1$ corresponds to infinite entanglement entropy, while $\xi = 0$ corresponds to decoupling

1. Positive coupling constant: $\alpha > 0$
   (a) $\omega_+ = 0 \Rightarrow \omega = 0$
   This corresponds to a zero mode.
   (b) $\omega_- \to \infty \Rightarrow \alpha \to \infty$
2. Negative coupling constant: $\alpha < 0$
   (a) $\omega_- = 0 \Rightarrow \alpha = -\dfrac{m\omega^2}{2}$
   This corresponds to a zero mode.
   (b) $\omega_+ = 0$ doesn't work, since then $\sqrt{\omega_-}$ is imaginary

3 Entanglement Entropy Calculations in Fock space

To look at this from a different perspective and try to understand the physical nature of the divergence in entanglement entropy, we solve the system in terms of the Fock space basis [5]. In this basis the energy eigenstates

Consider Eq(8). We define the creation and annihilation operators for the $\hat{x}_+$ and $\hat{x}_-$ Hilbert space as:

$$\hat{a}_+ = \frac{1}{\sqrt{2}}\left\{\sqrt{\frac{\hbar}{m\omega_+}}\hat{x}_+ + \iota\sqrt{\hbar m\omega_+}\hat{p}_+\right\} \; \hat{a}_+^\dagger = \frac{1}{\sqrt{2}}\left\{\sqrt{\frac{\hbar}{m\omega_+}}\hat{x}_+ - \iota\sqrt{\hbar m\omega_+}\hat{p}_+\right\} \tag{22}$$

$$\hat{a}_- = \frac{1}{\sqrt{2}}\left\{\sqrt{\frac{\hbar}{m\omega_-}}\hat{x}_- + \iota\sqrt{\hbar m\omega_-}\hat{p}_-\right\} \; \hat{a}_-^\dagger = \frac{1}{\sqrt{2}}\left\{\sqrt{\frac{\hbar}{m\omega_-}}\hat{x}_- - \iota\sqrt{\hbar m\omega_-}\hat{p}_-\right\} \tag{23}$$

following the bosonic commutation relations:

$$[\hat{a}_-, \hat{a}_-^\dagger] = [\hat{a}_+, \hat{a}_+^\dagger] = 1 \tag{24}$$

The Hamiltonian becomes:

$$\hat{H} = \hbar\omega_+ \hat{a}_+^\dagger \hat{a}_+ + \hbar\omega_- \hat{a}_-^\dagger \hat{a}_- + \frac{\hbar}{2}\{\omega_+ + \omega_-\} \tag{25}$$

The ground state of this Hamiltonian is given by:

$$|0\rangle = |0\rangle_+ \otimes |0\rangle_- \tag{26}$$

with the following action of the annihilation operators:

$$\hat{a}_\pm |0\rangle = 0 \tag{27}$$

Since the ground state is expressed in the $\pm$ basis, we cannot find the entanglement entropy for the individual harmonic oscillators. Therefore we need to express the ground state in terms of the Fock space states for the individual Hilbert spaces H_1(Hilbert space corresponding to x_1 harmonic oscillator) and H_2(Hilbert space corresponding to x_2 harmonic oscillator). i.e.:

$$|0\rangle = \sum_{n,m} C_{nm} |n\rangle_1 \otimes |m\rangle_2 \tag{28}$$

$|n\rangle_1$ corresponds to H_1 basis, and $|m\rangle_2$ corresponds to H_2 basis. To do so we first need to find the creation/annihilation operators confined to the individual Hilbert spaces which can be created with a linear combination of $\hat{a}_+$ and $\hat{a}_-$ operators.

Consider $\hat{a} = \frac{1}{\sqrt{2}}(\hat{a}_+ + \hat{a}_-)$ and $\hat{b} = \frac{1}{\sqrt{2}}(\hat{a}_+ - \hat{a}_-)$.

$$\hat{a} = \frac{1}{2}\left\{\sqrt{\frac{\hbar}{m\omega_+}}\hat{x}_+ + \iota\sqrt{\hbar m\omega_+}\hat{p}_+ + \sqrt{\frac{\hbar}{m\omega_-}}\hat{x}_- + \iota\sqrt{\hbar m\omega_-}\hat{p}_-\right\} \tag{29}$$

$$\begin{aligned}\hat{a} =& \frac{1}{2}\left\{(\sqrt{\frac{\hbar}{m\omega_+}} + \sqrt{\frac{\hbar}{m\omega_-}})\hat{x}_1 + (\sqrt{\frac{\hbar}{m\omega_+}} - \sqrt{\frac{\hbar}{m\omega_-}})\hat{x}_2 + \right.\\ & \left. \iota(\sqrt{\hbar m\omega_+} + \sqrt{\hbar m\omega_-})\hat{p}_1 + \iota(\sqrt{\hbar m\omega_+} - \sqrt{\hbar m\omega_-})\hat{p}_2\right\}\end{aligned} \tag{30}$$

After some algebra, we can write the equation as:

$$\hat{a} = \sqrt{\frac{\hbar}{1-\xi^2}}\left\{\sqrt{\frac{\omega}{2}}\left(\hat{x}_1 + \frac{\iota}{\omega}\hat{p}_1\right) - \xi\sqrt{\frac{\omega}{2}}\left(\hat{x}_2 - \frac{\iota}{\omega}\hat{p}_2\right)\right\} \tag{31}$$

$$\omega = m\sqrt{\omega_+\omega_-},\ \xi = \frac{\sqrt{\omega_-} - \sqrt{\omega_+}}{\sqrt{\omega_-} + \sqrt{\omega_+}}$$

Similarly we get:

$$\hat{b} = \sqrt{\frac{\hbar}{1-\xi^2}}\left\{\sqrt{\frac{\omega}{2}}\left(\hat{x}_2 + \frac{\iota}{\omega}\hat{p}_2\right) - \xi\sqrt{\frac{\omega}{2}}\left(\hat{x}_1 - \frac{\iota}{\omega}\hat{p}_1\right)\right\} \tag{32}$$

Take $\hat{\lambda} = \sqrt{\frac{\omega}{2}}\left(\hat{x}_1 + \frac{\iota}{\omega}\hat{p}_1\right)$ and $\hat{\mu} = \sqrt{\frac{\omega}{2}}\left(\hat{x}_2 + \frac{\iota}{\omega}\hat{p}_2\right)$. These follow the ladder operator commutation relations and hence we can define them as ladder operators confined to the H_1 and H_2 Hilbert spaces. This is important since this will help us in obtaining the ground state wave function in the required basis.

Therefore, $a = \sqrt{\frac{\hbar}{1-\xi^2}}\left\{\hat{\lambda} - \xi\hat{\mu}^\dagger\right\}$ and $b = \sqrt{\frac{\hbar}{1-\xi^2}}\left\{\hat{\mu} - \xi\hat{\lambda}^\dagger\right\}$

From Eq(27) we get: $\left\{\hat{\lambda} - \xi\hat{\mu}^\dagger\right\}|0\rangle = \left\{\hat{\mu} - \xi\hat{\lambda}^\dagger\right\}|0\rangle = 0$

$$\hat{\lambda}|0\rangle = \xi\hat{\mu}^\dagger|0\rangle \tag{33}$$

$$\hat{\mu}|0\rangle = \xi\hat{\lambda}^\dagger|0\rangle \tag{34}$$

From Eq(28) and standard action of ladder operators on the basis states we get:

$$\hat{\lambda}|0\rangle = \sum_{n,m=0}^{\infty} C_{nm}\sqrt{n}|n-1\rangle_1 \otimes |m\rangle = \sum_{n,m=0}^{\infty} C_{(n+1)m}\sqrt{n+1}|n\rangle_1 \otimes |m\rangle_2 \tag{35}$$

Similarly,

$$\xi\hat{\mu}^\dagger|0\rangle = \sum_{n,m=0}^{\infty} {}_{nm}\sqrt{m+1}|n\rangle_1 \otimes |m+1\rangle = \sum_{n,m=0}^{\infty} C_{n(m-1)}\sqrt{m}|n\rangle_1 \otimes |m\rangle_2 \tag{36}$$

Equating coefficients from Eq(35) and Eq(36), we get:

$$C_{(n+1)m}\sqrt{n+1} = \xi C_{n(m-1)}\sqrt{m} \tag{37}$$

Similarly,

$$C_{n(m+1)}\sqrt{m+1} = \xi C_{(n-1)m}\sqrt{n} \tag{38}$$

$$C_{nm} = \xi C_{(n-m)(m-1)}\sqrt{\frac{m}{n}} \tag{39}$$

$$C_{nm} = \xi C_{(n-1)(m-1)}\sqrt{\frac{n}{m}} \tag{40}$$

This gives us $C_{nm} \propto \xi^n \delta_{nm}$. By normalizing, we get:

$$C_{nm} = \sqrt{1-\xi^2}\xi^n\delta_{nm} \tag{41}$$

where $-1 < \xi < 1$. The ground state then becomes

$$|0\rangle = \sqrt{1-\xi^2}\sum_{n=0}^{\infty}\xi^n|n\rangle_1 \otimes |n\rangle_2 \tag{42}$$

From the form of the wavefunction in Fock space we can get the eigenvalues of the reduced density matrix as $p_n = (1-\xi^2)\xi^{2n}$

The entanglement entropy is given by:

$$S(\xi) = -\sum_{n=0}^{\infty} p_n \ln p_n = -\ln(1-\xi^2) - \frac{\xi^2}{1-\xi^2}\ln\xi^2 \tag{43}$$

The entanglement entropy (Eq(43)) diverges in the limit $\xi^2 \to 1$ (Fig. 2).

Again we look at two cases:

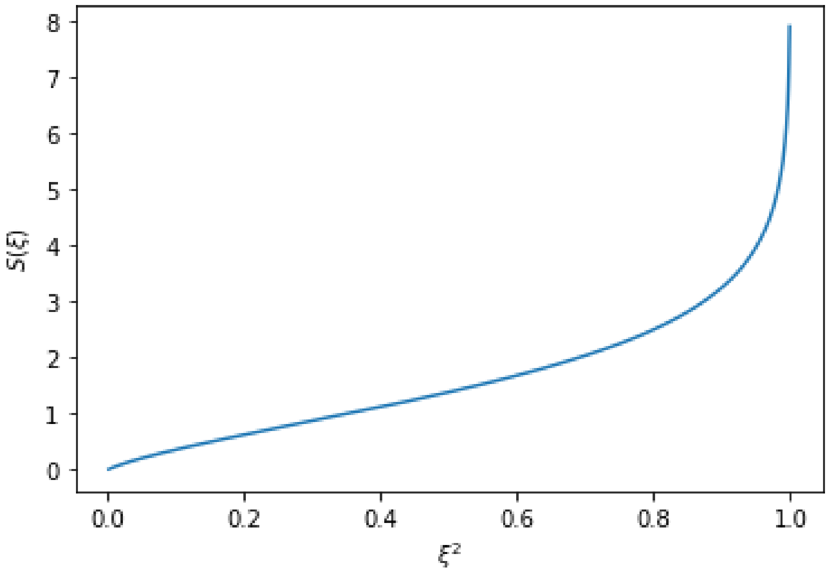


Figure 2: Entanglement energy for a coupled harmonic oscillator. $\xi^2 \to 1$ corresponds to infinite entanglement entropy, while $\xi^2 = 0$ corresponds to decoupling

1. Positive coupling constant $\alpha > 0$
   We again have two cases:

   (a) $\omega_+ = 0 \implies \omega = 0$
   This corresponds to a zero mode.

   (b) $\omega_- \to \infty \implies \alpha \to \infty$

   This gives us a ground state of the following form

$$|0\rangle \propto \sum_{n=0}^{\infty} |n\rangle_1 \otimes |n\rangle_2 \tag{44}$$

   Eq(44) shows that all states of the Fock space contribute equally to the divergence of the entanglement entropy. Further work needs to be done to understand the physical nature of these contributions.

2. Negative coupling constant $\alpha < 0$
   We have one case:

   (a) $\omega_- = 0 \implies \alpha = -\frac{m\omega^2}{2}$
   This corresponds to a zero mode.

   (b) $\omega_+ = 0$ doesn't work, since then $\sqrt{\omega_-}$ is imaginary

   This gives us a ground state of the following form

$$|0\rangle \propto \sum_{n=0}^{\infty} (-1)^n |n\rangle_1 \otimes |n\rangle_2 \tag{45}$$

Similr to Eq(44), Eq(45) shows that all states of the Fock space contribute equally to the divergence of the entanglement entropy, with alternting coefficients. Further work needs to be done to understand the physical nature of these contributions.

4 Entanglement Energy Calculation

To further understand the divergence of entanglement entropy, we calculate the entanglement energy for the system following reference [6]'s definition of entanglement energy:

$$E_{ent} = \langle : H_{in} : \rangle \tag{46}$$

where $: H_{in} :$ is the part of Hamiltonian dependent on the coordinates of one of the harmonic oscillators in normal order form.

$: H_{in} :$ can be written as:

$$: H_{in} := -\frac{1}{2}\delta^{ab}\left(\frac{\partial}{\partial x^a} - \omega^{in}_{ac}x^c\right)\left(\frac{\partial}{\partial x^b} + \omega^{in}_{bd}x^d\right) \tag{47}$$

where $\omega^{in} = \sqrt{K_{in}}$. Transforming to a new basis $\{\bar{x}^A\}$:

$$\bar{x}^A = \delta^{AB}(\Omega^{\frac{1}{2}})_{BC}x^C \tag{48}$$

$$U^{AB} = \delta^{AC}(\Omega^{\frac{1}{2}})_{Ca}\delta^{ab}(\Omega\frac{1}{2})_{bD}\delta^{DB} \tag{49}$$

$$\bar{\omega}^{in}_{AB} = \delta_{AC}(\Omega^{-\frac{1}{2}})^{Ca}\omega^{in}_{ab}(\Omega^{-\frac{1}{2}})^{bD}\delta_{DB} \tag{50}$$

The normal ordered Hamiltonian becomes:

$$: H_{in} := -\frac{1}{2}U^{ab}\left(\frac{\partial}{\partial \bar{x}^A} - \omega^{in}_{AC}\bar{x}^C\right)\left(\frac{\partial}{\partial \bar{x}^B} + \omega^{in}_{BD}\bar{x}^D\right) \tag{51}$$

The entanglement energy becomes:

$$E_{ent} = \int \prod_{A=1}^{N} d\bar{x}^A \langle\{\bar{x}^A\}| : H_{in} : \rho|\{\bar{x}^C\}\rangle \tag{52}$$

$$E_{ent} = \frac{1}{4}Tr[K_{in}\tilde{A} + A - 2\omega^{in}] \tag{53}$$

$$K_{in} = \begin{bmatrix} m^2\omega^2 + \alpha m & -\alpha m \\ -\alpha m & m^2\omega^2 + \alpha m \end{bmatrix} \tag{54}$$

$$\sqrt{K_{in}} = \begin{bmatrix} \sqrt{m^2\omega^2 + 2\alpha m} + m\omega & m\omega - \sqrt{m^2\omega^2 + 2\alpha m} \\ m\omega - \sqrt{m^2\omega^2 + 2\alpha m} & \sqrt{m^2\omega^2 + 2\alpha m} + m\omega \end{bmatrix} \tag{55}$$

Therefore, $A = \sqrt{m^2\omega^2 + 2\alpha m} + m\omega$, $\tilde{A} = \dfrac{\sqrt{m\omega^2 + 2\alpha m} + m\omega}{m\omega\sqrt{m^2\omega^2 + 2\alpha m}}$ and $\omega^{in} = \sqrt{m^2\omega^2 + \alpha m}$ [3].

$$E_{ent} = \frac{1}{8}\left[\left(\sqrt{\omega^2 + \frac{2\alpha}{m}} + \omega\right)\left(\frac{\omega^2 + \frac{\alpha}{m}}{\omega\sqrt{\omega^2 + \frac{2\alpha}{m}}} + 1\right) - 4\sqrt{\omega^2 + \frac{2\alpha}{m}} \right] \tag{56}$$

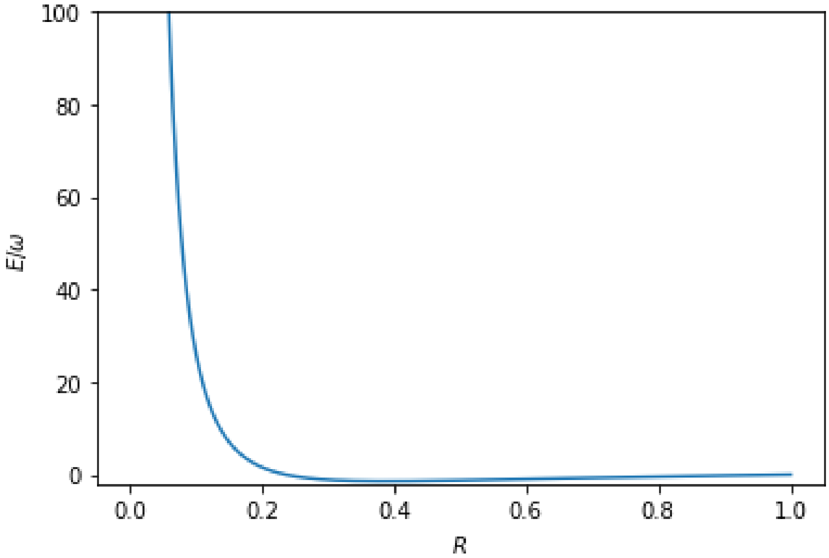
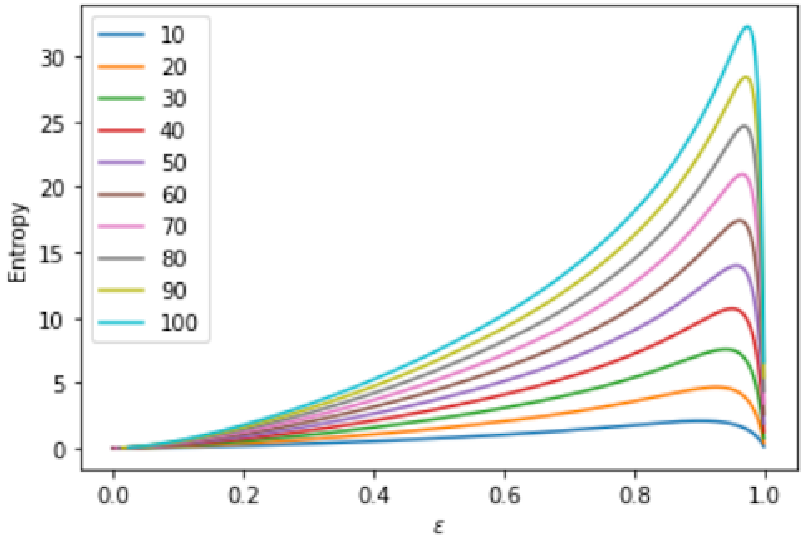


Figure 3: Entanglement energy for a coupled harmonic oscillator. $R = \frac{\omega_+}{\omega_-}$

5 Cut-off



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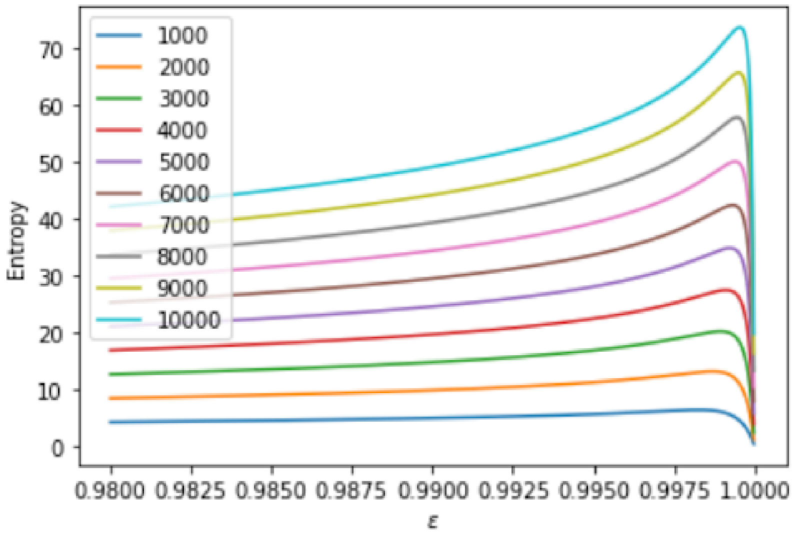
Entropy
ε



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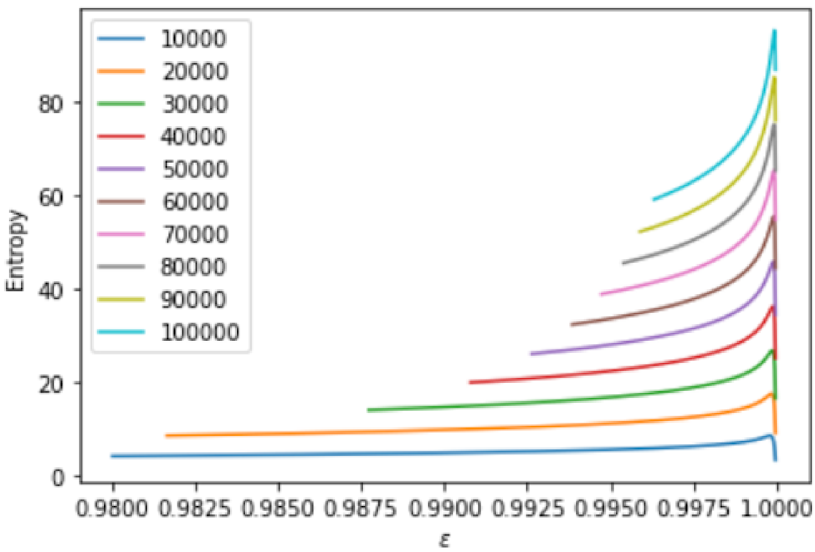

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6 Conclusion

We studied the divergence of entanglement entropy in a coupled harmonic oscillator with positive and negative coupling constants. We see that this divergence is a consequence of a zero mode in the harmonic oscillator system. This result is worked out in the coordinate space and Fock space basis. We also calculated the entanglement energy for the Hamiltonian (7) .

In the divergence limit, we find that ground state wavefunction has equal contributions from all the Fock space basis states (Eq(44) and Eq(45)). However we haven't grasped a physical understanding of these contributions. Such an understanding could help us in isolating the divergent contributions to the entanglement entropy.

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