

Bosonic Negative Energy Enhancement

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ABSTRACT: Wormholes are solutions to Einstein's equations connecting two different points of space-time. Traversable wormhole constructions, in which a particle can enter one side of the wormhole and exit through the other in a finite amount of time, require large amounts of negative energy. Recent progress has demonstrated that there exist physical systems that can produce this required amount of negative energy. In this work, motivated by the Casimir effect, we probe for other physical systems that might have this negative energy-producing property. Specifically, we investigate the minimum possible uniform energy density that can exist in a bosonic system. Technically, we numerically search for such states by varying temperature-like variables attached to each site of a chain of finite length. Future work will then scale this process from 1+1 dimensions up through 3+1 dimensions, determining the minimum possible uniform energy density in each.

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1 Introduction

It has recently been found that along a finite slab in $(3+1)\text{D}$, a massless Dirac field admits states with arbitrarily large amounts of negative energy with respect to the antiperiodic vacuum [1]. Technically, these states were found numerically by varying over the space of states on this slab. The key takeaway of [1] is that fermions in $(3+1)\text{D}$ admit states with arbitrarily large amounts of negative energy.

In this work, we search for the same sort of enhanced negative energy states, now for a bosonic massive free scalar field. Technically, in the lattice picture we search for states which have a uniform energy profile along a chain of N simple harmonic oscillators which are nearest neighbor coupled. Our search for such states is equivalent to searching over the space of states, as our density matrix takes the form:

$$\log \rho = - \sum_a \beta_a H_a + \text{const.}, \quad (1.1)$$

where H_a are the onsite Hamiltonians, and the β_a are parameters that we can vary (c.f. Appendix B). Thus, the search over states is equivalent to varying the β_a 's.

Numerically, we perform a gradient descent algorithm on the β_a 's, with a cost function which sets the energies along our chain to some constant value. In order to compute this energy gradient, one must invoke symplectic methods, and in particular formulate a notion of symplectic perturbation theory (c.f. Appendix A).

One can easily show that, given the definition of a symplectic transformation in equation A.1, the set of symplectic matrices forms a group under matrix multiplication. Thus, we follow the multiplicative perturbation scheme introduced in [2], as opposed to the usual additive perturbation scheme, as it naturally takes into account this property of symplectic transformations. The details of this perturbation scheme are reviewed in Appendix A.

Applications to Wormholes

Certain solutions to Einstein's field equations in General Relativity, specifically those of the traversable wormhole between two spacelike separated regions of spacetime, require the existence of large amounts of negative energy within the wormhole [3]. Thus, discovering physical states in a given physically reasonable quantum field theory (QFT) that have arbitrarily large amounts of negative energy helps to validate these wormhole constructions.

As a technical note, also mentioned in [1], the construction presently discussed does not discover states with $(2+1)\text{D}$ Poincaré invariance, which is required of states which support a traversable wormhole. This is simply because we did not impose such a condition within our numerical search, and thus it does not show up in our cost function. Thus, the results here only suggest that further work is required to determine whether physical states in this field theory can have arbitrarily large negative energy and the aforementioned Poincaré invariance.

Outline

The outline of this thesis is as follows. In section 2 we discuss the setup of our system, both in the field theory and lattice pictures. We then discuss the specific case of periodic conditions, which will be the scenario with respect to which we define our negative energy. We end section 2 with a brief comparison between the field theory and lattice pictures, which allows us to gain field theoretic intuition about the choices we make in the lattice picture. In section 3, we begin by motivating the use of symplectic methods in this model. We then expand on the numerical methods being used, and briefly mention the symplectic perturbation scheme. This scheme is more fully discussed in Appendix A. Finally,

in section 4, we discuss the results we have found in our analysis, as well as the key takeaways and interesting next steps.

2 Setup of the Problem and Energy Regulation

Consider a $(1+1)$ D bosonic massive free scalar field theory on an interval with unspecified boundary conditions. We wish to vary over all allowed states, and compare the ground state energy in each. Technically, this is most easily done by lattice regulating our field theory. Below we set up the field theory picture of our general system, and then consider the most general lattice realization. After this, we move on to analyze the specific case of periodic boundary conditions.

2.1 Field Theory Picture

Before describing our system as a field theory, we mention that we work in natural units within this thesis (i.e., $c = \hbar = 1$). Dimensionally, this means that position is equal to inverse momentum, that energy is equal to inverse time, and that position is equal to time. Also, throughout this thesis we will be using the mostly $-$ signature, which in $(1+1)$ D is $(+-)$ ¹.

The continuum picture of our system is described by a simple massive free scalar field with Lagrange density:

$$\mathcal{L} = \frac{1}{2}(\partial_t \varphi)^2 - \frac{1}{2}(\partial_x \varphi)^2 - \frac{m^2}{2}\varphi^2, \quad (2.1)$$

Our problem then becomes the following: given a $(1+1)$ D interval along this field theory, what is the minimum possible energy achievable when varying over the space of states. In order to obtain meaningful energies from our field theory, we must regulate it in some way, as it is well known that QFT calculations are riddled with infinities. For its ease of numerical implementation, we will be using a lattice regulation of our field theory, which simply means that we consider an analogous lattice system to our field theory which preserves the same physics. Such a lattice model is described below.

2.2 Lattice Picture

To numerically realize our system in $(1+1)$ D, we lattice regulate our field theory picture. That is, we consider N nearest neighbor interacting simple harmonic oscillators with an additional onsite term:

$$H = \sum_{i=1}^N \left[\frac{p_i^2}{2m} + \frac{1}{2}m\Omega^2 q_i^2 + \frac{\lambda}{2} \left((q_i - q_{i-1})^2 + (q_i - q_{i+1})^2 \right) \right] \quad (2.2)$$

Here, m is an onsite mass², λ is the coupling strength between nearest neighbors, and Ω is the frequency of onsite springs. An intuitive picture of this setup is seen in figure 1. As with the field theory picture, in the lattice picture we wish to vary over the states to find the minimum possible uniform energy density. This would correspond to varying over how site 1 is connected to site N .

¹It should be noted that this convention makes me just as nauseous and unwell as it would for any sane physicist. But, I promise it makes things easier– I’m not going to the dark side without reason.

²Note that this mass is different in general than the mass that appears in our field theory picture. As discussed in section 2.3.3, the frequency Ω of the onsite spring seen in figure 1 is equivalent to something like the mass of our field theory

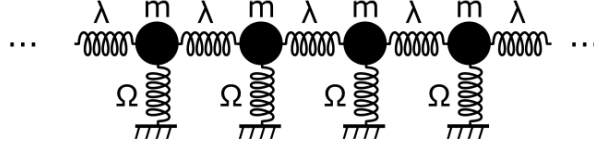


Figure 1. Simple picture of our lattice regulated field theory.

2.3 Periodic Boundary Conditions: This Again?

As mentioned extensively in the above sections, we would like to find the minimum possible energy in our system by varying over the allowed states on our slab. Before moving on to the general case, which is covered in sections 3 and 4, we will consider the special case of periodic boundary conditions. In both pictures, this is equivalent to connecting the two spatial ends of our $(1+1)$ D system into a circle.

The reason we care about the periodic boundary condition case is because this will be the setup with respect to which we define our negative energy. That is, if we find a state with energy less than that computed in the periodic boundary condition system, then we will consider this new state to have negative energy.

Through this example, we will learn about regulating the infinities that naturally appear in QFT, and about the connection between the field theory and lattice pictures.

2.3.1 Field Theory Picture

It is well known that a general solution to equation 2.1 subject to periodic boundary conditions is of the form:

$$\varphi(x) = \sum_k \left(c_k a_k e^{-ik \cdot x} + c_k^* a_k^\dagger e^{ik \cdot x} \right), \quad (2.3)$$

with $k = \frac{n}{R}$, where here $x = (t, x)$ and $k = (\omega, k)$ is a reduction of the usual 4-vector notation used in field theory to $(1+1)$ D. The equations of motion for equation 2.1 are found using the Euler-Lagrange equations:

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi)} = \frac{\partial \mathcal{L}}{\partial \varphi} \implies \partial_t^2 \varphi = \partial_x^2 \varphi - m^2 \varphi, \quad (2.4)$$

which, upon plugging in for equation 2.3, gives the dispersion relation:

$$\omega_k = \sqrt{k^2 + m^2}, \quad (2.5)$$

where again, imposing periodic boundary conditions, $k = \frac{n}{R}$, with $n \in \mathbb{N}$ and R the radius of the circle that our chain forms.

Calculating the minimum energy for this system (i.e., computing the ground state energy, which in Fock space is the state $|0, 0, \dots\rangle$), we find a divergent sum:

$$E_{gs}^{FT} = \sum_{n \in \mathbb{Z}} \frac{\omega_n}{2} = \sum_{n \in \mathbb{N}} \sqrt{\frac{n^2}{R^2} + m^2}, \quad (2.6)$$

where we have dropped the constant shift in energy provided by the $n = 0$ term in the sum³, since all we care about is differences in energies. In order to get a sensible answer, we must regulate this

³Yes, I define $0 \notin \mathbb{N}$, okay? It's the superior convention.

sum in some way, such that we can extract a universal and finite answer. Ideally, this finite part will be independent of the choice of regulator. Below we consider a few regulators, and show that they all give the same finite contribution to the ground state energy.

Setting $m = 0$

Setting $m = 0$ seems to be a harsh choice of regulator, as we are now considering a massless field, which naively would give a different ground state energy than a massive field. However, we may nonetheless compute the sum in equation 2.6. Doing so, the sum we wish to compute now becomes:

$$E_{gs}^{FT} = \frac{1}{R} \sum_{n \in \mathbb{N}} n, \quad (2.7)$$

which can be regulated using the Zeta function⁴. Thus, our ground state energy becomes:

$$E_{gs}^{FT} = -\frac{1}{12R}. \quad (2.8)$$

This is exactly what we wanted! We have obtained a finite answer for our previously divergent sum. We then hope that other choices of regulator will give a finite contribution to the ground state energy that is equal to that seen in equation 2.8. As a side note, the fact that this energy is negative is a phenomenon known as the Casimir effect, and which has been observed experimentally to occur (c.f. [4]).

For those who have not seen, or are uncomfortable with using, the Zeta function, we can equally tame the sum in equation 2.7 by setting $n \rightarrow ne^{-\epsilon n}$ in the limit $\epsilon \rightarrow 0$. Doing so, our sum becomes:

$$\sum_{n \in \mathbb{N}} ne^{-\epsilon n} = -\sum_{n \in \mathbb{N}} \partial_{\epsilon} e^{-\epsilon n} = -\partial_{\epsilon} \sum_{n \in \mathbb{N}} \left(\frac{1}{e^{\epsilon}}\right)^n = -\partial_{\epsilon} \left(\frac{1}{1 - e^{-\epsilon}}\right), \quad (2.9)$$

where we have used the linearity of the derivative and the geometric sum formula. Then, performing this derivative, we get that our total ground state energy is:

$$E_{gs}^{FT} = \frac{1}{R} \frac{e^{\epsilon}}{(e^{\epsilon} - 1)^2} = \frac{1}{2R} \frac{1}{\cosh(\epsilon) - 1}. \quad (2.10)$$

And, Laurent expanding this function about small ϵ , we find that:

$$E_{gs}^{FT} = \frac{1}{2R} \left(\frac{2}{\epsilon^2} - \frac{1}{6} + \frac{\epsilon^2}{120} + \mathcal{O}(\epsilon^4) \right), \quad (2.11)$$

where the finite term in the limit of $\epsilon \rightarrow 0$ is again $-\frac{1}{12R}$, as expected.

Setting $mR \rightarrow 0$.

This is a slightly less strict form of regulation than the $m = 0$ case we considered above. We are simply assuming we are in the limit of vanishing mass, or equivalently the limit of vanishing radius for our system. Either way, our ground state energy equation 2.6 in this limit (upon expanding the radical) becomes:

$$E_{gs}^{FT} = \frac{1}{R} \sum_{n \in \mathbb{N}} \left[n + \frac{m^2 R^2}{2n} + \frac{m^4 R^4}{8n^3} + \mathcal{O}(m^6 R^6) \right]. \quad (2.12)$$

⁴The Zeta function is given by $\zeta(s) = \sum_{n \in \mathbb{N}} n^{-s}$. So, we see here that we wish to compute $\zeta(-1)$, which has a known value of $-\frac{1}{12}$.

Thus, we can regulate the first and third term as we did above using the Zeta function⁵, and the second term we can regulate using the Ramanujan summation and the Cauchy principal value⁶:

$$\sum_{n \in \mathbb{N}} \frac{1}{n} = \gamma_E. \quad (2.13)$$

We can equally say that this term in equation 2.12 blows up, as one can argue that the Zeta function has a simple pole at $s = 1$. Either way, to leading order in mR , we see that the finite term in the ground state energy is given by $E_{gs}^{FT} = -\frac{1}{12R}$, as expected.

Power Series in mR

The final choice of regulator we will consider is a power series in mR , which is exact. That is, recall that the binomial theorem says that:

$$(x + y)^n = \sum_{k=0}^{\infty} \frac{\Gamma(n+1)}{\Gamma(k+1)\Gamma(n-k+1)} x^{n-k} y^k, \quad (2.14)$$

where here $\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t} dt$ is the usual gamma function. Using this, our ground state energy becomes:

$$E_{gs}^{FT} = \frac{1}{R} \sum_{n \in \mathbb{N}} \sqrt{n^2 + m^2 R^2} = \frac{1}{R} \sum_{n \in \mathbb{N}} \sum_{k=0}^{\infty} \frac{\Gamma(3/2)}{k! \Gamma(3/2 - k)} (mR)^{2k} n^{1-2k}. \quad (2.15)$$

Separating out the $k = 0$ and $k = 1$ terms, we find:

$$E_{gs}^{FT} = \frac{1}{R} \left[\sum_{n \in \mathbb{N}} n + \sum_{n \in \mathbb{N}} \frac{\Gamma(3/2)}{\Gamma(1/2)} \frac{(mR)^2}{n} + \sum_{n \in \mathbb{N}} \sum_{k=2}^{\infty} \frac{\Gamma(3/2)}{k! \Gamma(\frac{3}{2} - k)} (mR)^{2k} n^{1-2k} \right], \quad (2.16)$$

where we can regulate the first and third term using the zeta function, and we can regulate the second term using the Cauchy principal value method used above. Then, we get that our ground state energy is:

$$E_{gs}^{FT} = -\frac{1}{12R} + \frac{m^2 R^2}{2R} \gamma_E + \sum_{k=2}^{\infty} \frac{\Gamma(3/2)}{k! \Gamma(\frac{3}{2} - k)} (mR)^{2k} \zeta(2k - 1), \quad (2.17)$$

where here we swapped the order of sums in the third term and used the definition of the zeta function.

As expected, the leading order of this expression exactly agrees with our previous regulators, meaning we have found a universal, finite energy which is the physical energy of the system, which should be the same regardless of choice of regulator. Thus, we choose to use the lattice regulator, as our above analysis suggests that it should still give the same finite contribution to the ground state energy.

Before proceeding, we note how the above analysis fits into our solution. We have shown above that we can regulate our field theory such that we extract a finite, physical energy (this is the $-\frac{1}{12R}$ that we kept finding). Then, what we want to do is to find a state such that even this finite, physical energy can be arbitrarily negative. So, the enhanced negative energy that we are finding is not the product of a lack of regulator. Instead, it is a novel statement about subsystems of a field theory.

⁵Where here the term proportional to n is regulated by $\zeta(-1)$ and the term proportional to n^{-3} is regulated by $\zeta(3)$.

⁶The cauchy principal value of a function $f(x)$ at x is given by $\lim_{\epsilon \rightarrow 0} \frac{f(x+\epsilon) + f(x-\epsilon)}{2}$.

2.3.2 Lattice Picture

We begin with our Hamiltonian given in equation 2.2, and we impose periodic boundary conditions. That is, we have a chain of N nearest neighbor interacting particles. We start by assuming a purely classical system. Then, using Hamilton's equation, we get that the equations of motion are:

$$m\ddot{q}_j = -(m\Omega^2 + 4\lambda) q_j + 2\lambda q_{j+1} + 2\lambda q_{j-1}, \quad (2.18)$$

which, upon imposing periodic boundary conditions, is solved by:

$$q_n(t) = Ae^{-i\omega t - ikna}, \quad (2.19)$$

for a the lattice spacing (i.e., the distance between sites on our lattice). As we've invoked periodic boundary conditions, this solution is invariant under the shift $k \rightarrow k + \frac{2\pi}{a}$, meaning we may set $k = k_n = \frac{2\pi n}{Na}$. Then, plugging this solution into equation 2.18, and using the above invariance of k , we get:

$$-m\omega^2 q_n = -(m\Omega^2 + 4\lambda) q_n + 2\lambda q_{n+1} + 2\lambda q_{n-1} = -(m\Omega^2 + 4\lambda) q_n + 2\lambda q_n e^{-ika} + 2\lambda q_n e^{ika}. \quad (2.20)$$

So, our dispersion relation is:

$$\omega = \omega_n = \sqrt{\Omega^2 + \frac{8\lambda}{m} \sin^2\left(\frac{ka}{2}\right)} = \sqrt{\Omega^2 + \frac{8\lambda}{m} \sin^2\left(\frac{\pi n}{N}\right)}. \quad (2.21)$$

So far, we've considered only a classical system. Quantizing our results, subject to the commutation relations:

$$[\hat{q}_n, \hat{p}_{n'}] = i\delta_{nn'}, \quad (2.22)$$

we get a solution:

$$\hat{q}_n(t) = \sum_l \left(\hat{A}_l e^{-i(\omega_l t - k_l na)} + \hat{A}_l^\dagger e^{i(\omega_l t - k_l na)} \right). \quad (2.23)$$

Then, using the usual definition of the position and momentum operators:

$$\hat{q}_i = \frac{1}{\sqrt{2m\omega}} \left(a_i^\dagger + a_i \right) \quad \hat{p}_i = i\sqrt{\frac{m\omega}{2}} \left(a_i^\dagger - a_i \right), \quad (2.24)$$

we find that finding the quantum mechanical energy expectation value, $\langle H \rangle_0 \equiv \langle 0 | H | 0 \rangle$, from 2.2, is:

$$E_{gs}^{Lat} = \sum_{n=1}^{N/2} \left(\frac{\omega_n}{2} + \frac{\Omega^2}{2\omega_n} + \frac{2\lambda}{m\omega_n} \right). \quad (2.25)$$

Thus, we have found the ground state energy⁷ of our (now quantum mechanical) lattice regulation of our field theory. Let's take a slight (but beneficial) detour and discuss what we have found.

⁷This is an energy. Later in section 3.2 we are computing energy densities. So, in section 4 when we plot our preliminary results, we must divide the above analytic solution for the energy by the number of sites.

2.3.3 Lattice vs Field Theory vs Brown vs The Board of Education

Above we have found that the ground state energy for our field theory is given by equation 2.6, whereas that for our lattice regulated field theory is given by equation 2.25. The lattice energy should equal the field theory energy in the limit of large N , such that Na is held constant. Moreover, in this limit the two dispersion relations, given by equations 2.21 and 2.5, should also be equal. Taking this limit, we find the following:

$$\omega_k^{Lat} \approx \sqrt{\Omega^2 + \frac{8\lambda}{m} \frac{\pi^2 n^2}{N^2}}, \quad (2.26)$$

Comparing this equation with the form of the field theory dispersion relation, equation 2.5, we find that, in the limit of large N , these two pictures agree when we set $\Omega = m_{FT}$ and $R = \frac{N}{2\pi} \sqrt{\frac{m}{2\lambda}}$. And, since we know that the length of our slab in the field theory picture is proportional to Na , where a is the lattice spacing, we see that we further set $a = \sqrt{\frac{m}{2\lambda}}$. The extra 2π in our formula for R is an artifact of interchanging between R being the radius and circumference of the circle that our system forms when imposing periodic boundary conditions.

That is, we have found that the onsite spring in our lattice model is something like the mass in our field theory, which is a useful tool to help build intuition between these two pictures. Moreover, by equating these two dispersion relations in a certain limit, we have found for free that the length of our slab in the field theory is equal to the number of sites times the lattice spacing in the lattice picture, and we have found a formula for the lattice spacing.

Now that we have discussed the periodic boundary conditions system, let's remove this rather stringent constraint. In the next section, we will build up the methods necessary to probe over arbitrary states on our slab.

3 Methods

Now that we have setup our problem, and have considered the special case of periodic boundary conditions, we may now move on to the more general case. In this section, we discuss the methods necessary in order to complete our analysis. In the last part of this section, we also develop a perturbation theory on symplectic eigenvalues, which is vital in our solution.

3.1 Why Symplectic?

In section 1, we mentioned that our system of interest is solved using the notion of symplectic transformations. We will now briefly describe why this is.

In the limiting case of $N = 1$, we see that our Hamiltonian simplifies to something like:

$$H = \frac{1}{2} (Ap^2 + Bx^2), \quad (3.1)$$

for some constants of the system A and B . The key observation here is that equation 3.1 looks like a harmonic oscillator. What we'd like to do now is to make this vague observation more obvious. So, let's consider the mapping $x \rightarrow \lambda x = \tilde{x}$ and $p \rightarrow \frac{1}{\lambda} p = \tilde{p}$, where $\lambda \in \mathbb{R}^\times$. Then, our Hamiltonian maps to:

$$H = \frac{1}{2} \left(A\lambda^2 \tilde{p}^2 + \frac{B}{\lambda^2} \tilde{x}^2 \right). \quad (3.2)$$

Upon assuming that $\lambda^2 = \sqrt{\frac{B}{A}}$, we find that our Hamiltonian is:

$$H = \frac{\sqrt{AB}}{2} (\tilde{p}^2 + \tilde{x}^2), \quad (3.3)$$

where $\frac{1}{2}(\tilde{p}^2 + \tilde{x}^2)$ is the harmonic oscillator with $\omega = m = 1$, and thus has a spectrum of $(n + \frac{1}{2})$. Thus, we have found a transformation which has taken our initial Hamiltonian 3.1 to something that is diagonal in the $\{x, p\}$ basis of the form $d_i I_2$, as in equation 3.3, where I_2 is the 2×2 identity. Such a transformation is provided from Williamson's theorem, and thus is symplectic (c.f. Appendix A).

Thus, moving to arbitrary N inductively, we see that symplectic transformations will play a crucial role in diagonalizing our Hamiltonian.

3.2 Computing Energies

It was shown in [5] that for a given lattice theory, if there is a state with some distribution of energy, there must exist a state, with the same energy distribution, which maximizes the von Neumann entropy $-\text{Tr}\{\rho \log \rho\}$. We know that such a state must take the form:

$$\rho = \frac{1}{Z} e^{-\sum_a \beta_a H_a}, \quad (3.4)$$

for some parameters β_a (c.f. Appendix B).

Clearly from equation 3.4, we see that our energies will depend on β_a . To numerically compute the energies, we start with the partition function derived in Appendix B. We know that $H = \sum_a \beta_a H_a$ is a positive definite, real, $2N \times 2N$ matrix, and so is subject to Williamson's theorem. Thus, there exists a symplectic matrix S that transforms SHS^T to a direct sum of harmonic oscillators. That is:

$$SHS^T = \bigoplus_{i=1}^N d_i \left(\frac{1}{2} \tilde{x}^2 + \frac{1}{2} \tilde{p}^2 \right). \quad (3.5)$$

Thus, our partition function becomes:

$$Z = \text{Tr} \left\{ e^{-\sum_a \beta_a H_a} \right\} \rightarrow \sum_{\{n_i\}} \prod_i e^{-d_i (n_i + \frac{1}{2})} \quad (3.6)$$

$$= \prod_{i=1}^N e^{-d_i/2} \sum_{n_i=0}^{\infty} e^{-d_i n_i}, \quad (3.7)$$

where in equation 3.6 we use that the spectrum of $(\frac{1}{2} \tilde{x}^2 + \frac{1}{2} \tilde{p}^2)$ is $n_i + \frac{1}{2}$, for n_i the usual occupation number at site i . In equation 3.7, we use ∞ for the upper bound of the occupation number because we are considering a bosonic system. Then, using the usual geometric sum rule on equation 3.7, we get that our partition function is:

$$Z = \prod_i \frac{e^{-d_i/2}}{1 - e^{-d_i}}, \quad (3.8)$$

where d_i are the symplectic eigenvalues of H .

Next, let's derive the onsite energy in our system. Well, at a site a , the energy E_a is related to the partition function via $E_a = \frac{d}{d\beta_a} (-\ln Z)$. Then, using equation 3.8:

$$E_a = \frac{d}{d\beta_a} \left[\sum_i \left(\frac{d_i}{2} - \ln(1 - e^{-d_i}) \right) \right] = \frac{d}{d\beta_a} \left[\sum_i \left(d_i - \ln \left(2 \cosh \frac{d_i}{2} \right) \right) \right] = \frac{d}{d\beta_a} \sum_i h_0(d_i). \quad (3.9)$$

It then follows, from the functions defined in Appendix C, that we can write:

$$E_a = \sum_i h_1(d_i) \frac{d}{d\beta_a} d_i. \quad (3.10)$$

But, what is this $\frac{d}{d\beta_a}d_i$ quantity? Well, this is precisely the first order perturbative correction to the i th symplectic eigenvalue of the matrix $M = M_0 + gV = H + gH^a$, for some small parameter g . Thus, defining $\frac{d}{d\beta_a}d_i \equiv d_{i,a}^{(1)}$, we see that our onsite energy is given by:

$$E_a = \sum_i h_1(d_i) d_{i,a}^{(1)}, \quad (3.11)$$

where $d_{i,a}^{(1)}$ is defined in section 3.4 below.

3.3 Gradient Descent

Since from equation 3.11 we see that the onsite energies do in fact depend on our β_a 's, to minimize our energy, we may wish to numerically search over the space of states by varying $\{\beta_a\}$. As a brief aside, we wish to clarify that varying over $\{\beta_a\}$ is in fact varying the state of our system. We saw above that the state of our system is given by equation 3.4:

$$\rho = \frac{1}{Z} e^{-\sum_a \beta_a H_a}, \quad (3.12)$$

which clearly shows that by varying over $\{\beta_a\}$ we are varying over the state of our system. And, now that we have introduced these onsite parameters β_a , we may consider an altered Hamiltonian, which will be the weighted sum of onsite Hamiltonians:

$$H = \sum_a \beta_a H_a, \quad (3.13)$$

where each H_a is a term in the sum of equation 2.2. We are considering 3.13 to be our new Hamiltonian instead of 2.2 because we wish to find a true minimum energy for our system, where we only hold fixed the size of our slab. But, by varying $\{\beta_a\}$, and thus varying 3.13, we aren't actually changing the boundary conditions of our system. This is simply because some configurations of our state don't have a boundary condition interpretation, and so we can only consider them on an open chain. Then, we would really consider our slab to have some (possibly mixed) state, which is then purified by the outside physics⁸. However, we don't care about this outside physics, so it suffices to only change the state.

To ensure that a given set $\{\beta_a\}$ produces a physical state, we can require that we minimize the cost function:

$$C(\beta, \vec{E}) = \frac{1}{2} \sum_a (\text{Tr}\{\rho(\beta) H_a\} - E_a^{set})^2 = \frac{1}{2} \sum_a (E_a - E_a^{set})^2, \quad (3.14)$$

where here $\vec{E}^{set} = (E_1^{set}, \dots, E_N^{set})$ is the set of energies that we are fixing. But, we are specifically looking for uniform energy profiles. Then, to numerically find a minimum of our energy, we can proceed using a gradient descent algorithm, subject to the constraint that our energy density profile is uniform. That is, we use the cost function:

$$C_U = \frac{1}{2} \sum_a (E_a - E^{set})^2, \quad (3.15)$$

for some fixed E^{set} . Following [1], we will set E^{set} to the energy of the middle site(s) of our chain, and we will initially set these β to be much larger than the others along the chain. And, when updating

⁸One possible set of purifications is simply identifying the ends of the slab with periodic or antiperiodic boundary conditions. However, often the purifications are not amenable to such boundary condition interpretations, and instead describe some non-trivial physics outside the slab.

the β parameters, we do not update β_{mid} . As an aside, the reason that this sets a true minimum in our chain is because, when we set β_{mid} to be large, we are finding E_{mid} in the limit $T \rightarrow 0$. In words, this 0 temperature limit is truly the lowest energy that one can achieve. So, since our cost function sets all other energies equal to this true minimum energy, we are guaranteed to find a uniform minimum energy profile when minimizing the cost function⁹. And, when β_{mid} is large enough, E_{mid} is independent of the other choices of β_a , as the H_{mid} term will dominate in the Hamiltonian 3.13.

To reiterate, we know that minimizing the cost function 3.15 has to do with minimizing the resultant uniform energy density because we hand select β_{mid} such that E_{mid} is the true $T \rightarrow 0$ ground state energy. We then optimize the other β_a such that our energy profile is uniform, where each energy is being set to this $T \rightarrow 0$ limit of E_{mid} . Moreover, we choose to set the middle energy to the $T \rightarrow 0$ limit because this site on our chain is the most insensitive to the physics outside of our slab. This is important because, for large enough N , we can assume that the energy we select in the middle of the chain is not only in the $T \rightarrow 0$ limit, but also in the $N \rightarrow \infty$ limit, meaning it is in fact the vacuum ground state energy for $T \rightarrow 0$.

Thus, at each step of the gradient descent, we update our parameters using the rule:

$$\beta_a \rightarrow \beta_a - \alpha \frac{\partial C_U}{\partial \beta_a}, \quad (3.16)$$

where as usual α is some learning rate that we choose to maximize the efficiency of our algorithm. In order to compute the gradient $\frac{\partial C_U}{\partial \beta_a}$, we must find the gradient of the energies. That is, we see that:

$$\frac{\partial C_U}{\partial \beta_b} = \sum_a (E_a - E^{set}) \frac{dE_a}{d\beta_b}. \quad (3.17)$$

The gradient of energy is computed explicitly in Appendix C, where we find that:

$$\frac{dE_a}{d\beta_b} = \sum_i h_2(d_i) \frac{dd_i}{d\beta_a} \frac{dd_i}{d\beta_b} + \sum_i h_1(d_i) \frac{\partial^2 d_i}{\partial \beta_a \partial \beta_b}. \quad (3.18)$$

We already saw above in section 3.2 that $\frac{dd_i}{d\beta_a}$ is equivalent to the first order perturbative correction to the i th symplectic eigenvalue of the total Hamiltonian perturbed by the a th onsite Hamiltonian. From equation 3.18 we see that we must make sense of $\frac{\partial^2 d_i}{\partial \beta_a \partial \beta_b}$. The correct interpretation of this derivative is that it is the second order perturbative contribution to the i th symplectic eigenvalue of the total Hamiltonian perturbed by the a th and b th onsite Hamiltonians via some small parameters g_a and g_b , respectively. This can readily be seen by expanding out the definition of the derivative.

Thus, we have found that $\frac{\partial^2 d_i}{\partial \beta_a \partial \beta_b} \equiv d_{i,a,b}^{(2)}$. Next, let's develop a perturbation scheme on symplectic eigenvalues, since these seems to be vital in our current analysis¹⁰.

3.4 Perturbation Theory on Symplectic Eigenvalues

Suppose we have a $2N \times 2N$ real positive definite matrix $M = M_0 + gV$, for some small parameter g , and we wish to perturbatively solve for the symplectic eigenvalues of M . Then, utilizing Williamson's

⁹Since the energy saturates exponentially in β (which can be found by recalling that the energy of a simple harmonic oscillator is proportional to the average occupation number, which itself can be written in terms of an inverse exponential using Bose-Einstein statistics.

¹⁰After searching the literature, there seemed to be no concrete method of computing perturbative corrections to symplectic eigenvalues to first and second order. Thus, section 3.4 is a novel extension of the work in [2], where we offer analytic formulas for the first and second order perturbative corrections to symplectic eigenvalues.

theorem on M , and equation A.5:

$$(S_0 + gBS_0 + g^2CS_0 + \dots)(M_0 + gV)(S_0^T + gS_0^TB^T + g^2S_0^TC^T + \dots) = \bigoplus_{j=1}^N \left(d_j^{(0)} + gd_j^{(1)} \dots \right) I_2, \quad (3.19)$$

where I_2 is the usual 2×2 identity matrix, and $d_j^{(i)}$ is the i th perturbative correction to the j th symplectic eigenvalue.

Next, we can match either side of equation 3.19 in powers of g . To 0th order, we get the usual statement of Williamson's theorem:

$$S_0 M_0 S_0 = \bigoplus_{j=1}^N d_j^{(0)} I_2. \quad (3.20)$$

To 1st order in g , though, we get a more interesting result:

$$BS_0 M_0 S_0^T + S_0 V S_0^T + S_0 M_0 S_0^T B^T = \bigoplus_{j=1}^N d_j^{(1)} I_2 \quad (3.21)$$

And, to 2nd order in g , we get the equation:

$$CS_0 M_0 S_0^T + BS_0 V S_0^T + BS_0 M_0 S_0^T B^T + S_0 V S_0^T B^T + S_0 M_0 S_0^T C^T = \bigoplus_{j=1}^N d_j^{(2)} I_2. \quad (3.22)$$

We next wish to solve for the first and second order perturbative contributions to a given symplectic eigenvalue of M . Before proceeding, though, we must permute our symplectic matrices such that Williamson's theorem reads:

$$S'_0 M_0 S'_0 = D^{(0)} = \begin{pmatrix} \Lambda^{(0)} & 0 \\ 0 & \Lambda^{(0)} \end{pmatrix}, \quad (3.23)$$

where here $\Lambda^{(0)}$ is an $N \times N$ diagonal matrix of the N $d_j^{(0)}$'s. Such a permutation matrix is straightforwardly found to be constructed by the rule that, on the i th row of our permutation matrix σ , the only nonzero element lies on the j th column, where $j = N + \frac{i}{2}$ when i is even and $j = \frac{i+1}{2}$ when i is odd. With this permutation, Williamson's theorem takes the form of equation 3.23 when we set:

$$S'_0 = \sigma^T S_0. \quad (3.24)$$

Throughout the rest of this section we will assume that we have already multiplied by this σ .

Then, using equation 3.20, equation 3.21 becomes, in component form:

$$B_{ik} D_{kj}^{(0)} + P_{ij} + D_{ik}^{(0)} (B^T)_{kj} = D_{ij}^{(1)}, \quad (3.25)$$

where here and the rest of this section we will use Einstein's summation convention¹¹, and we define $P \equiv S_0 V S_0^T$. Then, assuming $i = j$ here, and not summing over a repeated i , we find that equation 3.25 becomes:

$$2B_{ii} d_i^{(0)} + P_{ii} = d_i^{(1)}. \quad (3.26)$$

We learned in appendix A that equation A.6 implies that, as blocks, $B_{11} = -B_{22}^T$. Thus, noting that $D_{ii}^{(0)} = D_{i+N, i+N}^{(0)}$, we can shift the i index in equation 3.26 by N , assuming $i \leq N$, to get:

$$-2B_{ii} d_i^{(0)} + P_{i+N, i+N} = d_i^{(1)}. \quad (3.27)$$

¹¹That is, a repeated index in a given term is assumed to be summed over.

Finally, adding equations 3.26 and 3.27, and solving for $d_i^{(1)}$:

$$d_{i,a}^{(1)} = \frac{P_{ii} + P_{i+N,i+N}}{2}. \quad (3.28)$$

Thus, we have found a formula for the first order perturbative correction to symplectic eigenvalues. Here, the a in the subscript was added to remind us that, for the problem at hand, the P matrix is constructed from the a th onsite Hamiltonian, as this is our perturbing matrix.

Now, we wish to find the second order perturbative correction. In order to do this, though, equation 3.22 tells us that we need to know the form of B . To compute components of B , it's as simple as using the symmetry properties of B from equation A.6, along with equation 3.25 when $i \neq j$. Combining these, it's straightforward to find, for $i \neq j$ and $i, j \leq N$:

$$B_{ij} = \frac{d_j^{(0)} P_{ij} + d_i^{(0)} P_{i+N,j+N}}{\left(d_i^{(0)}\right)^2 - \left(d_j^{(0)}\right)^2}, \quad (3.29)$$

$$B_{i+N,j} = \frac{d_i^{(0)} P_{i,j+N} - d_j^{(0)} P_{i+N,j}}{\left(d_j^{(0)}\right)^2 - \left(d_i^{(0)}\right)^2} \quad (3.30)$$

$$B_{i,j+N} = \frac{d_j^{(0)} P_{i,j+N} - d_i^{(0)} P_{i+N,j}}{\left(d_i^{(0)}\right)^2 - \left(d_j^{(0)}\right)^2}, \quad (3.31)$$

and for $i = j \leq N$, we find that:

$$B_{ii} = \frac{P_{i+N,i+N} - P_{ii}}{4d_i^{(0)}}. \quad (3.32)$$

The above equations give all of the contributing components of B . One may notice that we have not defined the diagonal elements of the off-diagonal blocks of B . This is because there is actually no closed form solution for these elements. This corresponds to some freedom on our choice of B , where this freedom lies along the diagonal elements of the off-diagonal blocks because J has its non-zero elements along these components.

Assuming that C has a block form, equation A.7 tells us that $C_{11} + C_{22}^T = B_{11}^2 + B_{12}B_{21}$. Using this formula, we can get rid of the C 's in equation 3.22, allowing us to write the second order perturbative contribution to our symplectic eigenvalues as:

$$d_{i,a,b}^{(2)} = d_i^{(0)} \left((B_{11}^2)_{ii} + (B_{12}B_{21})_{ii} \right) + (P_{ik}B_{ik} + P_{i+N,k}B_{i+N,k}) + \frac{1}{2}d_k^{(0)} \left((B_{ik})^2 + (B_{i+N,k})^2 \right), \quad (3.33)$$

where we are only summing over k . Here, the a, b subscripts were added to remind us that, generally, we consider $d_i^{(0)}$ to be the i th symplectic eigenvalue of the matrix $M = M_0 + g_a V_a$ (no sum over a), where for us $M_0 = H$ is the total Hamiltonian, $V_a = H_a$ is our first perturbing onsite Hamiltonian, and g_a is some small parameter. Then, P is constructed with the second perturbing matrix V_b , which for us is H_b . The reason we consider M to be already perturbed above is because of our analysis in 3.3, where we saw that $d_{i,a,b}^{(2)}$ corresponds to the second derivative $\frac{\partial^2 d_i}{\partial \beta_a \partial \beta_b} \equiv \frac{\partial}{\partial \beta_b} \frac{\partial d_i}{\partial \beta_a}$. Thus, we perturb an already perturbed matrix¹².

Now that we have formulated our numerical methods, let's consider our results.

¹²As a note, the analysis just presented is symmetric in swapping a and b , as the partial derivatives commute with each other.

4 Results and Discussions

We now have all of the necessary tools to perform our calculation. Preliminary results, found by minimizing our cost function using a gradient-free optimization algorithm, show that there do in fact exist states with energy less than that of a state with periodic boundary conditions. These results are seen in figure 2. Although these data are incredibly noisy (in part due to the brute force algorithm not converging for certain Ω), we see clear evidence for the existence of states that have enhanced negative energy. To clarify, these energies (the orange points) are enhanced simply because they are less than the energies of states with the same Ω where periodic boundary conditions are imposed (the blue points for numerical results or the green line for analytic results).

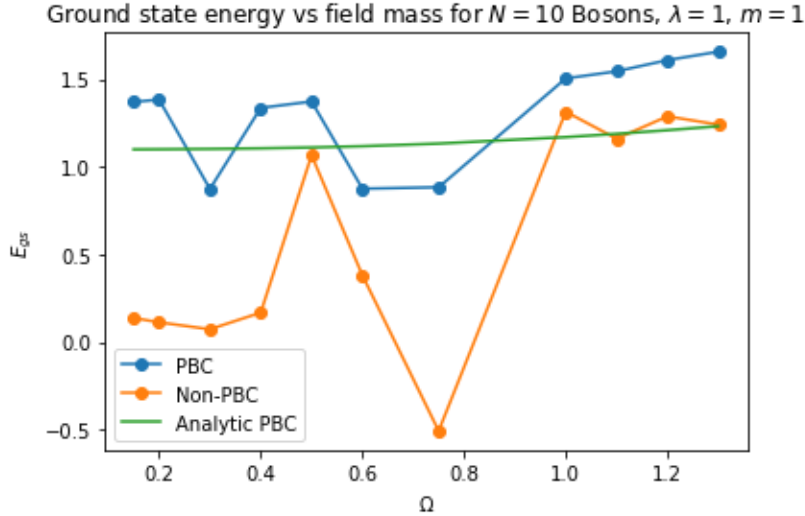


Figure 2. Numerical evidence of negative energy enhancement in 1D on a chain of length $N = 10$. The blue data points are made from performing our optimization algorithm over the β_{as} for the Hamiltonian 3.13 with additional terms that impose periodic boundary conditions. The orange data points are made from performing our optimization algorithm over the β_{as} for the Hamiltonian 3.13 as it is, without any additional boundary conditions. The green line is the analytic ground state energy for a system with PBC, from 2.25. We have selected $\lambda = 1$, $m = 1$.

A useful plot to discuss the validity of the numerical results in figure 2 is figure 3. We see that, on figure 3, the points where the blue data is closest to the green analytic line in figure 2, we have relatively small cost function values for the PBC system. And, points where the non-PBC system energy either goes negative (which is impossible here, since our Hamiltonian is positive definite) or is larger than the analytic PBC energy (which should not happen if we truly have energy enhancement), the associated cost function values are two orders of magnitude larger than those of the other, likely more accurate, energies. And, the fact that these two scenarios – the non-PBC becoming negative and being larger than the analytic PBC energy – have cost function values of the same order of magnitude, they are both likely not reasonable results. We know for sure that the negative energy result is inconsistent with our Hamiltonian, and so we can deduce that the points where our non-PBC energy is greater than that of the analytic PBC system are also inconsistent. Thus, figure 3 gives further evidence that our enhanced energy states are valid.

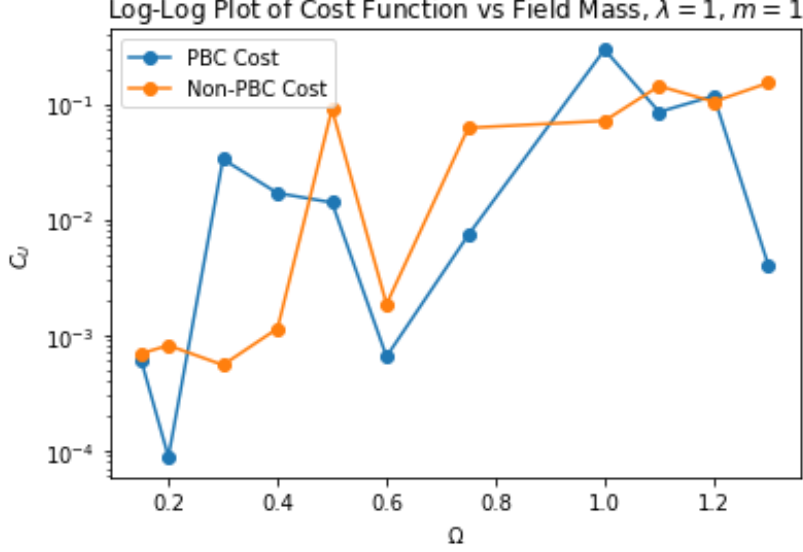


Figure 3. Cost function (3.15) values for the numerical data shown in figure 2, plotted on a log-log plot due to the large range of values. A smaller cost function value corresponds to a more accurate corresponding energy value in figure 2. The blue and orange data correspond to those in figure 2.

We are working on find an analytic expression for the second order perturbative contribution to symplectic eigenvalues. Once we find this, our numerical implementation will increase in speed greatly.

After we find the minimum possible negative energy by implementing this gradient descent algorithm, the process would proceed as follows. We would perform this minimization of the energy for various Ω , which in 2.3.3 we saw is equivalent to the field theory mass. Then, we would find the power law relationship between the minimum energy and Ω . That is, suppose we find that the optimized ground state energy that we find scales as Ω^p . Then, in the fashion of [1], a massless bosonic field of sufficiently high dimension would have a UV sensitive ground state energy.

To clarify, suppose we find that our optimized ground state energy scales as Ω^p . Then, we would consider a $(d+1)$ D massless bosonic field, with $d-1$ transverse dimensions having on-shell momenta. That is, each transverse direction can itself be considered a $(1+1)$ D bosonic field with mass given by the corresponding on-shell momentum. Each momentum is on-shell (or, can be considered a mass) because the transverse dimensions are not on a slab, but are translation invariant. Thus, their contribution to the field are of the form $e^{ik_{\perp} \cdot z_{\perp}}$, multiplied by the $(1+1)$ D field along the slab, where k_{\perp} are the transverse momenta and z_{\perp} are the transverse directions. Our (now massless) $(d+1)$ D field theory, described by:

$$\mathcal{L} = \frac{1}{2} (\partial_t \varphi)^2 - \frac{1}{2} (\nabla \varphi)^2, \quad (4.1)$$

picks up an extra factor of $-\frac{k_{\perp}^2}{2} \phi^2$, which looks like a mass. The reason, for sufficiently large d , that we have a UV sensitive optimized ground state energy is because our energy goes as:

$$\int dk_{\perp}^{d-1} |k_{\perp}|^p. \quad (4.2)$$

Thus, what we have found is that, if our power law relationship in the $(1+1)$ D case has a power of $p > 1-d$, then our $(d+1)$ D energy is clearly UV sensitive. Thus, the corresponding states in

our $(d + 1)$ D field theory carry negative energy that can be arbitrarily negative, since our energy is unbounded when taking the limit of large mass cutoff.

It would be interesting to consider the above analysis with two additional, physical constraints. Firstly, the states we search for above are not physically allowed states within a wormhole construction, so we would firstly want to impose a $(2 + 1)$ D Poincaré invariance, which would guarantee that our states are physical. Secondly, it would be interesting to impose the constraint that our states are stationary. That is, that the T_{zz} component of our energy momentum tensor is also uniform across the chain.

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A Symplectic Methods

In this appendix we review the main definitions and theorems of symplectic transformations that show up throughout this thesis. For a more complete review of these methods, see [2, 6, 7], and all the references therein. Everything in this Appendix is either directly from or a corollary of the methods in [2, 6, 7].

A.1 Symplectic Transformations

To start, we begin by constructing symplectic transformations. To do so, we must first define a symplectic form:

Definition 1 *Let V be a real vector space. Then, a **symplectic form** on V is a mapping $\omega : V \times V \rightarrow \mathbb{R}$ which is bilinear and antisymmetric in its entries, and also non-degenerate.*

Given any symplectic form, we can combine a real vector space with this form to form a symplectic space, as defined below:

Definition 2 *A **real symplectic space** is a pair (V, ω) , with V a real vector space on \mathbb{R} and ω a symplectic form.*

Finally, with this definition of real symplectic spaces, we can construct the group of symplectic transformations:

Definition 3 *The set of all symplectic automorphisms $S : (E, \omega) \rightarrow (E, \omega)$ forms a multiplicative group, $Sp(E, \omega)$ satisfying:*

$$SJS^T = J, \tag{A.1}$$

where we choose J , in block-diagonal form, to be:

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{A.2}$$

with I being the $N \times N$ identity matrix. More generally, J is just some $2N \times 2N$ antisymmetric, invertible matrix.

This machinery on its own is quite beautiful, and can be seen as a generalization of orthogonality. That is, the statement of orthogonality is that $OO^T = I$ for some matrix, O , or rather $OIO^T = I$. Thus, a symplectic matrix is seen to be the case where we replace the usual identity matrix, I , with some invertible, antisymmetric matrix, J .

A.2 Williamson's Theorem

When considering symplectic transformations, we find a slightly different form of diagonalization which in the current analysis is indispensable:

Theorem 1 (*Williamson's Theorem*) *Let M be a positive-definite, real, $2N \times 2N$ matrix. Then, there exists a symplectic transformation, S , such that:*

$$SMS^T = D, \quad (\text{A.3})$$

where

$$D = \bigoplus_{j=1}^N d_j \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (\text{A.4})$$

where for all j , $d_j > 0$. This set of numbers $\{d_j\}$ is known as the set of symplectic eigenvalues of M .

A very accessible proof of this theorem is found in [6].

A.3 Symplectic Perturbation Theory

It is known that perturbation theory on symplectic matrices is more easily done using a multiplicative perturbation structure, as opposed to the usual additive structure [2]. Thus, if we are perturbing a symplectic matrix, S , in some small parameter g , we write the perturbative series as:

$$S(g) = (I + gB + g^2C + \mathcal{O}(g^3)) S_0, \quad (\text{A.5})$$

which is natural when realizing the multiplicative nature of the symplectic structure¹³. We also know that in order for $S(g)$ to be symplectic, B must satisfy the following equation [2]:

$$BJ + JB^T = 0, \quad (\text{A.6})$$

and further that C must satisfy:

$$CJ + JC^T + BJB^T = 0. \quad (\text{A.7})$$

Supposing that B is a block diagonal matrix, of the form $B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$. Then, equation A.6 is equivalent to saying that $B_{11} = -B_{22}^T$ and that B_{12} and B_{21} are symmetric.

B Entropy Maximizing States

Given some state on a lattice with energy distribution (E_1, \dots, E_N) , there always exists a von Neumann entropy maximizing state with the same energy distribution [5]. We would like to find the form of this entropy-maximizing state, ρ . Then, for a given set of onsite H_a subject to the constraint that

¹³Specifically, that the symplectic matrices form a group under matrix multiplication.

the expectation value of H_a is E_a , we see that, in order to find ρ , we must extremize the equation of constraint:

$$-\text{Tr}\{\rho \log \rho\} - \sum_a \beta_a (\text{Tr}\{\rho H_a\} - E_a) - \gamma (\text{Tr}\{\rho\} - 1), \quad (\text{B.1})$$

where $\{\beta_a\}$ and γ are Lagrange multipliers. The second term above sets the expectation value of each H_a to be E_a , while the third term above sets the normalization condition for our density matrix ρ . Thus, extremizing equation B.1 by demanding a vanishing variation:

$$-\text{Tr}\{\delta \rho \log \rho - \delta \rho\} - \sum_a \beta_a \text{Tr}\{\delta \rho H_a\} - \gamma \text{Tr}\{\delta \rho\} = 0 \quad (\text{B.2})$$

$$\text{Tr}\left\{\delta \rho \left(\log \rho - 1 + \sum_a \beta_a H_a + \gamma\right)\right\} = 0. \quad (\text{B.3})$$

As equation B.3 holds for arbitrary $\delta \rho$, we find that our state ρ must satisfy:

$$\log \rho = - \sum_a \beta_a H_a + \text{const.}, \quad (\text{B.4})$$

meaning our ρ takes the form:

$$\rho = e^{-\sum_a \beta_a H_a} e^{\text{const.}}. \quad (\text{B.5})$$

And, imposing the constraint that ρ is properly normalized, we find that:

$$e^{\text{const.}} = \frac{1}{Z(\beta)} = \frac{1}{\text{Tr}\{e^{-\sum_a \beta_a H_a}\}}. \quad (\text{B.6})$$

Thus, our final entropy-maximizing state is:

$$\rho = \frac{1}{Z(\beta)} e^{-\sum_a \beta_a H_a}, \quad (\text{B.7})$$

where $Z(\beta)$ is our partition function.

C Useful Functions for Energy Gradient

We saw in section 3.2 that

$$E_a = \frac{d}{d\beta_a} \sum_i h_0(d_i). \quad (\text{C.1})$$

We wish to pass the derivative through the sum. Doing so, we define the following functions (following closely the notation of [1]):

$$h_0(d_i) = d_i - \ln(2 \cosh(d_i/2)) \quad (\text{C.2})$$

$$h_1(d_i) \equiv h'_0(d_i) = 1 - \frac{\sinh(d_i/2)}{2 \cosh(d_i/2)} = \frac{1}{2} (2 - \tanh(d_i/2)) \quad (\text{C.3})$$

$$h_2(d_i) \equiv h'_1(d_i) = -\frac{1}{4} (1 - \tanh^2(d_i/2)). \quad (\text{C.4})$$

Then, passing the derivative through the sum, we find that:

$$E_a = \sum_i h_1(d_i) \frac{dd_i}{d\beta_a} \quad (\text{C.5})$$

In section 3.3, we note that we wish to compute $\frac{dE_a}{d\beta_b}$. Using equation C.5:

$$\frac{dE_a}{d\beta_b} = \sum_i h_2(d_i) \frac{dd_i}{d\beta_a} \frac{dd_i}{d\beta_b} + \sum_i h_1(d_i) \frac{\partial^2 d_i}{\partial \beta_a \partial \beta_b}, \quad (\text{C.6})$$

where these first and second derivatives are defined in section 3.4.

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