

# **Prototyping many-body approximations in quantum computing**

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(Dated: June 30, 2021)

I discuss how to apply several common approximations to the Lipkin model, in the context of quantum computing: mean-field theory, projected mean-field theory, and generator coordinate methods.

## I. THE LIPKIN MODEL

The Lipkin model has  $N$  particles, each of which is in one of two states. Thus each particle is interpreted as having spin-1/2 (though they are not fermions—the particles are in principle distinguishable) and the single-particle states having  $m = \pm 1/2$ . We label the states by  $i, \uparrow, i, \downarrow$ . The Hamiltonian is thus usually written in quasispin formalism,

$$\hat{\mathcal{H}} = -\epsilon \hat{J}_z - \frac{1}{2} V (\hat{J}_+^2 + \hat{J}_-^2). \quad (1)$$

Here we write

$$\hat{J}_z = \frac{1}{2} \sum_{i=1}^N \hat{a}_{i,\uparrow}^\dagger \hat{a}_{i,\uparrow} - \hat{a}_{i,\downarrow}^\dagger \hat{a}_{i,\downarrow}, \quad (2)$$

$$\hat{J}_+ = \sum_i \hat{a}_{i,\uparrow}^\dagger \hat{a}_{i,\downarrow}, \quad (3)$$

$$\hat{J}_- = (\hat{J}_+)^{\dagger} = \sum_i \hat{a}_{i,\downarrow}^\dagger \hat{a}_{i,\uparrow}. \quad (4)$$

Although there are  $2^N$  many-body states, one can use the quasispin formalism to reduce this down to a problem of size  $\sim N/2$ .

The simplicity and the ease of full solution of the Lipkin model makes it a good pedagogical testbed for many-body approximations.

*Note:* the first term of Eq. (1) has a - sign relative to the way it is normally written. This does not matter, because the Lipkin model is symmetric under that change, but it allows us to keep other intuition.

### A. Solving the Lipkin model

The Lipkin Hamiltonian commutes with  $\hat{J}^2$ , hence we can use  $|j, m\rangle$  as a basis. Because the maximum  $m = \frac{N}{2}$  we conclude that the maximum  $j_{\max} = \frac{N}{2}$  as well. It turns out that the ground state always belongs to this  $j_{\max}$ . However it is possible later when looking at excited states we will have to consider  $j < j_{\max}$ .

In the basis  $|j, m\rangle$ , we can compute the matrix elements of the Hamiltonian. We do that by using

$$\hat{J}_z |j, m\rangle = m |j, m\rangle, \quad (5)$$

$$\hat{J}_{\pm} |j, m\rangle = \sqrt{j(j+1) - m^2 \mp m} |j, m \pm 1\rangle, \quad (6)$$

the latter which comes from SU(2) commutation relations. The only nonzero matrix elements are

$$\langle j, m | \hat{H} | j, m \rangle = \epsilon m, \quad (7)$$

$$\begin{aligned} \langle j, m+2 | \hat{H} | j, m \rangle &= -\frac{V}{2} \sqrt{[j(j+1) - m(m+1)]} \\ &\quad \times \sqrt{[j(j+1) - (m+1)(m+2)]}. \end{aligned} \quad (8)$$

Before going further, we can deduce some properties of the quantum numbers. We do this much in the same way as we did for the seniority Hamiltonian. For example, the extremal possible values of  $m$  are either  $N/2$  (all states  $\uparrow$ ) or  $-N/2$  (all  $\downarrow$ ). Thus, for a given  $N$ , the maximal value of  $j$  must be  $N/2$ .

Second, because the interaction is of the form  $\hat{J}_+^2 + \hat{J}_-^2$ , which either promotes two particles from  $\downarrow$  to  $\uparrow$  or demotes two from  $\downarrow$  to  $\uparrow$ , we can define a conserved ‘parity’, which is  $(-1)^{N_{\uparrow}}$ . That is, the Hamiltonian will connect two many-body states, both of which have either an even number of up particles or an odd number of up particles, but will never connect an even number of up particles with an odd number of up particles. This is reflected in the matrix element (8), which connects states that differ in  $m$  by 2 but not by 1.

So, for a given  $j$ , there are two separate sets of solutions: those constructed from states with  $m = j, j-2, j-4, \dots$  and those with  $m = j-1, j-3, \dots$

Furthermore, for a given  $N$ , the possible  $j$ s are  $N/2, N/2-1, N/2-2, \dots$ . This can be confusing, because it means systems with  $N$  particles have a spectrum that includes the energies for  $N-2$  particles,  $N-4$  particles, etc.. This

arises because of the simple, semi-algebraic nature of the Hamiltonian, but is not unknown in more realistic systems: in nuclei we have *isospin analogs* found in neighboring isobars (nuclei with the same  $A = Z + N$  but different  $Z, N$ ).

Let's consider a specific case:  $N = 3$ , so that the maximal  $j = 3/2$  and the possible  $j$ s are  $3/2, 1/2$ . For simplicity we set  $\epsilon = 1$ . For  $j = 1/2$ , the Hamiltonian is trivial:

$$\mathbf{H}_{j=1/2} = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}. \quad (9)$$

For  $j = 3/2$  the Hamiltonian matrix is slightly more interesting:

$$\mathbf{H}_{j=3/2} = \begin{pmatrix} 3/2 & 0 & -\sqrt{3}V & 0 \\ 0 & 1/2 & 0 & -\sqrt{3}V \\ -\sqrt{3}V & 0 & -1/2 & 0 \\ 0 & -\sqrt{3}V & 0 & -3/2 \end{pmatrix}. \quad (10)$$

and we see that we get either  $m = 3/2, -1/2$  (which we label as “odd parity” although it has no physical meaning aside from having an odd number of particles “up”) or  $m = 1/2, -3/2$  (even parity). We can solve for the eigenvalues exactly, and get  $E = 1/2 \pm \sqrt{1 + 3V^2}$  for odd parity solutions and  $E = -1/2 \pm \sqrt{1 + 3V^2}$  for even solutions.

For larger  $N$ , of course, one must diagonalize numerically. An example for  $N = 20$  is in Fig. 1.

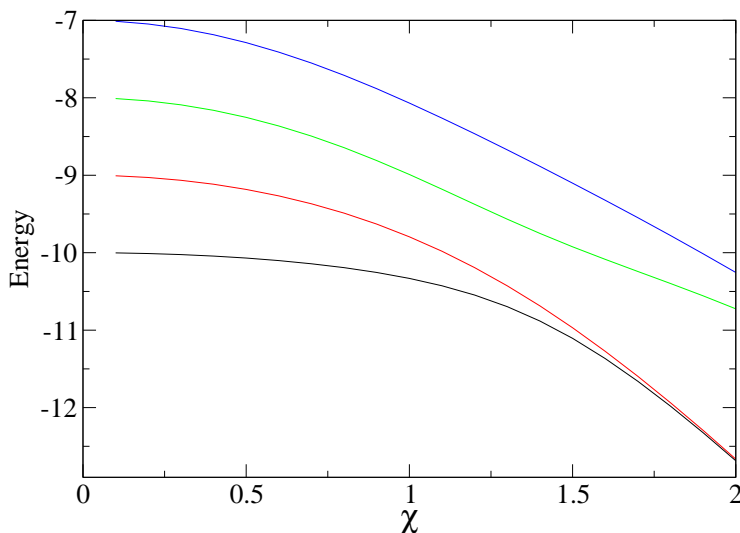


FIG. 1. Ground state and first three excited states of the Lipkin model with  $N = 20$ ,  $\epsilon = 1$ , though exact diagonalization .

Another example is given below in Fig. 2.

## II. THE UNIFORM APPROXIMATION: INSPIRED BY THE MEAN FIELD

The first approximation is a simple variational approximation, akin to Hartree-Fock (HF), although it is not solved in exact analogy to HF. One posits a trial wave function which is a simple product wave function, akin to a Slater determinant, albeit without antisymmetry as the particles are distinguishable:  $|\Psi_T\rangle = \prod_{i=1}^N \hat{c}_i^\dagger |0\rangle$ . Furthermore, I assume

$$\hat{c}_i^\dagger(\theta) = \hat{a}_{i,\uparrow}^\dagger \cos \theta + \hat{a}_{i,\downarrow}^\dagger \sin \theta, \quad (11)$$

so that  $\theta = 0$  corresponds to all particles in the  $\uparrow$  state. (This is the consequence of the - sign in front of the first term in Eq. (1). The reason for this choice is that in quantum computing,  $|\uparrow\rangle$  corresponds to the qubit state  $|0\rangle$  which

is the usual default starting state.) For simplicity, I adopt the uniform approximation, that  $\theta$  is the same for all  $i$ , writing,

$$|\theta\rangle = \prod_{i=1}^N \hat{c}_i^\dagger(\theta)|0\rangle, \quad (12)$$

Note this is normalized, that is,

$$\langle\theta|\theta\rangle = (\langle 0|\hat{c}(\theta)\hat{c}^\dagger(\theta)|0\rangle)^N = 1. \quad (13)$$

This makes evaluation easy. So for example,

$$\langle\hat{J}_z\rangle = \frac{1}{2} \sum_{i=1}^N \langle\theta|\hat{a}_{i,\uparrow}^\dagger\hat{a}_{i,\uparrow} - \hat{a}_{i,\downarrow}^\dagger\hat{a}_{i,\downarrow}|\theta\rangle \quad (14)$$

$$= \frac{1}{2} \sum_{i=1}^N \langle 0|\hat{c}_i(\theta) \left( \hat{a}_{i,\uparrow}^\dagger\hat{a}_{i,\uparrow} - \hat{a}_{i,\downarrow}^\dagger\hat{a}_{i,\downarrow} \right) \hat{c}_i^\dagger(\theta)|0\rangle \quad (15)$$

$$= N \frac{1}{2} (\cos^2 \theta - \sin^2 \theta) = \frac{N}{2} \cos 2\theta \quad (16)$$

Similarly,

$$\langle\theta|\hat{J}_+^2 + \hat{J}_-^2|\theta\rangle = N(N-1)2\sin^2\theta\cos^2\theta = \frac{N(N-1)}{2}\sin^2 2\theta. \quad (17)$$

This means

$$\langle\hat{\mathcal{H}}\rangle = -\frac{N\epsilon}{2}\cos 2\theta - \frac{N(N-1)V}{4}\sin^2 2\theta = -\frac{N\epsilon}{2} \left[ \cos 2\theta + \frac{(N-1)V}{2\epsilon}\sin^2 2\theta \right] \quad (18)$$

Because of this, we introduce  $\chi = (N-1)V/\epsilon$  as the only nontrivial parameter of the theory. We can find the minimum easily,

$$\frac{\partial}{\partial\theta}\langle\hat{\mathcal{H}}\rangle = -N\epsilon[-\sin 2\theta + \chi\sin 2\theta\cos 2\theta] = 0 \quad (19)$$

which has solutions at either  $\theta = 0$  or  $\cos 2\theta = 1/\chi$ . For  $\chi < 1$ , we can only have the former, and for  $\chi > 1$ , the former is unstable (you can see that by taking the second derivative) and so must take the latter solution.

From this one can write analytically the “mean-field” approximation to the ground state energy:

$$E \approx \begin{cases} -\frac{N\epsilon}{2}, & \chi \leq 1; \\ -\frac{N\epsilon}{4} \left( \chi + \frac{1}{\chi} \right), & \chi \geq 1. \end{cases} \quad (20)$$

These of course agree at  $\chi = 1$ . An example comparing this ‘mean-field’ approximation with the exact diagonalization is shown in Fig. 2.

Note: we have to be careful here and throughout on notation. In particular we have to distinguish carefully the number of particles in a wavefunction. To that end I use the notation  $|\theta\rangle_n$  to denote  $n$  particles, so that  $|\theta\rangle_1 = \hat{c}^\dagger(\theta)|0\rangle$ ,  $|\theta\rangle_2 = \hat{c}_1^\dagger(\theta)\hat{c}_2^\dagger(\theta)|0\rangle$ , and so on. Thus, we write

$$\langle\hat{\mathcal{H}}\rangle_N = -N\epsilon\langle\hat{J}_z\rangle_1 - \frac{1}{2}VN(N-1)\langle\hat{J}_+^2 + \hat{J}_-^2\rangle_2. \quad (21)$$

**Exercise:** write a code to reproduce Fig. 2.

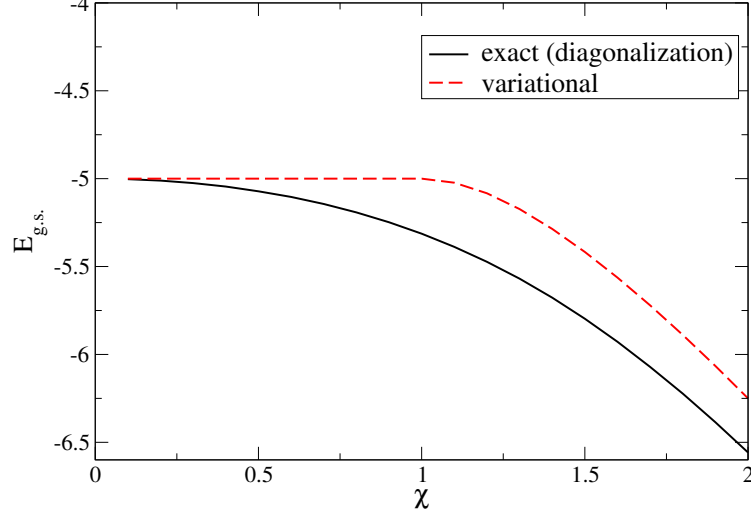
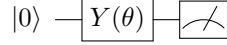


FIG. 2. Ground state of the Lipkin model with  $N = 10$ , both through exact diagonalization of the Hamiltonian (solid black line) and through the variational approximation (dashed red line).

### A. Implementation in a quantum circuit

The circuit to measure  $\langle \hat{J}_z \rangle$  is



The  $Y(\theta) = \exp(i\theta\mathbf{Y})$  gate rotates the qubit  $|0\rangle = |\uparrow\rangle$  to  $\cos(\theta/2)|0\rangle + \sin(\theta/2)|1\rangle$ , (**note: this is wrong for this definition of  $\mathbf{Y}(\theta)$ !** yet it is exactly what we want....) and  $|1\rangle$  to  $\cos(\theta/2)|1\rangle - \sin(\theta/2)|0\rangle$ . (Note: need to fix factor of 2, check if this definition is consistent with elsewhere, especially Qiskit.)

Indeed, we should use

$$\mathbf{R}_y(\theta) = \exp\left(-i\frac{\theta}{2}\mathbf{Y}\right) = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}. \quad (22)$$

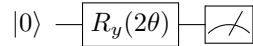
In Qiskit this is written as `u3( $\theta, 0, 0$ )`. The quantum truth table is

$$\mathbf{R}_y(\theta)|0\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)|1\rangle, \quad (23)$$

$$\mathbf{R}_y(\theta)|1\rangle = \cos(\theta/2)|1\rangle - \sin(\theta/2)|0\rangle. \quad (24)$$

In this definition, a single particle state  $|\theta\rangle = \hat{c}^\dagger(\theta)|0\rangle = \mathbf{R}_y(2\theta)|0\rangle$ .

The correct circuit measure  $\langle \hat{J}_z \rangle$  is



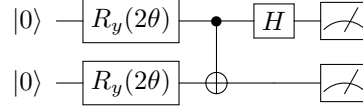
The probability to measure in the  $|0\rangle$  state is  $\cos^2 \theta$  while that to measure in the  $|1\rangle$  state is  $\sin^2 \theta$ , hence over many measurements

$$\langle \hat{J}_z \rangle = \frac{1}{2} (p(0) - p(1)) = p(0) - \frac{1}{2} = \frac{1}{2} \cos 2\theta. \quad (25)$$

To measure  $\langle \hat{J}_+^2 + \hat{J}_-^2 \rangle$ , we need to transform to a basis where  $\hat{J}_+^2 + \hat{J}_-^2$  is diagonal. In the usual order of the 2-qb basis, that is,  $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ , the representation of  $\hat{J}_+^2 + \hat{J}_-^2$  is

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad (26)$$

which has Bell states as eigenvectors:  $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$  has eigenvalue 1, while  $\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$  has eigenvalue -1, and the remaining Bell states have eigenvalue 0. To measure  $\hat{J}_+^2 + \hat{J}_-^2$ , therefore, we just decode the 2qb state from Bell states using a standard decoder:



If we measure  $|00\rangle$ , then we were in the first Bell state with eigenvalue +1, and if we measure  $|10\rangle$  we were in second Bell state with eigenvalue -1. Therefore

$$\langle \theta | \hat{J}_+^2 + \hat{J}_-^2 | \theta \rangle_2 = p(00) - p(10) \quad (27)$$

which should be  $\frac{1}{2} \sin^2 2\theta$ .

### III. VARIATION AFTER PROJECTION

The Lipkin model has a symmetry, namely the eigenstates are either even or odd in the number of  $\uparrow$  states. You can think of this as a kind of parity. The variational solution with  $\theta \neq 0$  violates this symmetry, but we can project out a state of good symmetry.

Because  $\sin \theta$  is odd in  $\theta$  and  $\cos \theta$  is even, then  $|\theta\rangle \pm |-\theta\rangle$ , for nonzero  $\theta$  is either even or odd. Therefore we compute the projected energy,

$$\frac{(\langle \theta | \pm \langle -\theta |) \hat{\mathcal{H}} (|\theta\rangle \pm |-\theta\rangle)}{(\langle \theta | \pm \langle -\theta |) (|\theta\rangle \pm |-\theta\rangle)} = \frac{\langle \theta | \hat{\mathcal{H}} | \theta \rangle \pm \langle -\theta | \hat{\mathcal{H}} | -\theta \rangle}{1 \pm \langle -\theta | \theta \rangle}, \quad (28)$$

where I've used  $\langle -\theta | -\theta \rangle = \langle \theta | \theta \rangle = 1$ , and  $\langle -\theta | \hat{\mathcal{H}} | -\theta \rangle = \langle \theta | \hat{\mathcal{H}} | \theta \rangle$ . The remainder is straightforward to evaluate. First, for one particle,

$$\langle 0 | \hat{c}_i(-\theta) \hat{c}^\dagger(+\theta) | 0 \rangle_1 = \cos^2 \theta - \sin^2 \theta = \cos 2\theta, \quad (29)$$

which means for  $N$  particles  $\langle -\theta | \theta \rangle_N = \cos^N 2\theta$ .

Next, let's compute the matrix elements  $\langle -\theta | \hat{\mathcal{H}} | \theta \rangle_N$ , term by term:

$$\langle 0 | \hat{c}(-\theta) \left( \hat{a}_\uparrow^\dagger \hat{a}_\uparrow - \hat{a}_\downarrow^\dagger \hat{a}_\downarrow \right) \hat{c}^\dagger(\theta) | 0 \rangle_1 = \cos^2 \theta + \sin^2 \theta = +1, \quad (30)$$

but when we include the overall normalization (expanded details to be added), we get

$$\langle -\theta | \hat{J}_z | \theta \rangle_N = \frac{N}{2} \cos^{N-1} 2\theta. \quad (31)$$

To get the rest of the Hamiltonian, we need to do some additional development in the next section.

### IV. GENERATOR COORDINATE

We can introduce a more general solution,

$$|\Psi\rangle = \int f(\theta') |\theta'\rangle d\theta'. \quad (32)$$

Then we get a generalized Schrödinger equation

$$\int f(\theta') \langle \theta | \hat{\mathcal{H}} | \theta' \rangle f(\theta') d\theta' = E \int f(\theta') \langle \theta | \theta' \rangle f(\theta') d\theta' \quad (33)$$

(In nuclear physics, the continuous parameter, here  $\theta$ , is often associated with an observable, such as quadrupole deformation, that is treated as a generalized coordinate; furthermore one “generates” the state through a constrained variational calculation. Hence the name, “generator coordinate.”) In practice, one discretizes this integral equation, and one can just think of it as using a small subset of nonorthogonal basis states to construct the wave function.

What's crucial is calculating the Hamiltonian and norm or overlap kernels, that is,  $\langle \theta | \hat{\mathcal{H}} | \theta' \rangle$  and  $\langle \theta | \theta' \rangle$ , respectively. This is not much harder than for the parity-projected case.

We can compute the correct result analytically. We need the overlap kernel

$$\langle \theta | \theta' \rangle_N = (\cos \theta \cos \theta' + \sin \theta \sin \theta')^N = (\cos(\theta - \theta'))^N, \quad (34)$$

and the elements of the Hamiltonian kernel, specifically,

$$\langle \theta | \hat{J}_z | \theta' \rangle_N = \frac{N}{2} \cos^{N-1}(\theta - \theta') (\cos \theta \cos \theta' - \sin \theta \sin \theta') = \frac{N}{2} \cos^{N-1}(\theta - \theta') \cos(\theta + \theta'), \quad (35)$$

and

$$\langle \theta | \hat{J}_+^2 + \hat{J}_-^2 | \theta' \rangle_N = N(N-1) \cos^{N-2}(\theta - \theta') (\cos^2 \theta \sin^2 \theta' + \cos^2 \theta' \sin^2 \theta). \quad (36)$$

Hence

$$\langle \theta | \hat{H} | \theta' \rangle_N = -\frac{N\epsilon}{2} \cos^{N-2}(\theta - \theta') [\cos(\theta - \theta') \cos(\theta + \theta') + \chi (\cos^2 \theta \sin^2 \theta' + \cos^2 \theta' \sin^2 \theta)] \quad (37)$$

### A. Back to parity-projection

When  $\theta' = \theta$  this reduces to our initial results. When  $\theta' = -\theta$  we get

$$\langle -\theta | \theta \rangle_N = \cos^N 2\theta, \quad (38)$$

$$\langle -\theta | \hat{J}_z | \theta \rangle_N = \frac{N}{2} \cos^{N-1} 2\theta, \quad (39)$$

and

$$\langle -\theta | \hat{J}_+^2 + \hat{J}_-^2 | \theta \rangle = N(N-1) \cos^{N-2}(2\theta) \frac{1}{2} \sin^2 2\theta. \quad (40)$$

From this one can work out the positive- and negative-parity projected “mean-field” energies:

$$E_{\pm}(\theta) = -\frac{N\epsilon}{2} \left[ \cos 2\theta + \frac{(N-1)V}{2\epsilon} \sin^2 2\theta \right] \frac{1 \pm \cos^{N-2}(2\theta)}{1 \pm \cos^N(2\theta)}. \quad (41)$$

I believe that one must find the minimum numerically. Note, however, for large  $N$ , for any  $\theta > 0$ , the correction terms get very small.

The projection is shown in Fig. 3. Interestingly, for large  $\chi$ , the mean-field and projected mean-field solutions all go to the same energy.

**Exercise:** Numerically find the minimum for the projected mean-field Lipkin solution, and plot against the exact solution, and the unprojected mean-field (as in Fig. 2).

### B. Solving the generator coordinate wave function

To solve the generator coordinate problem, one has to discretize the Hill-Wheeler integral and evaluate on a grid of  $\theta, \theta'$ . That is, construct a grid of angles  $\{\theta_i\}$ . Compute

$$\mathcal{N}_{i,j} = \langle \theta_i | \theta_j \rangle_N = (\cos(\theta_i - \theta_j))^N,$$

and

$$\mathcal{H}_{i,j} = -\frac{N\epsilon}{2} \cos^{N-2}(\theta_i - \theta_j) [\cos(\theta_i - \theta_j) \cos(\theta_i + \theta_j) + \chi (\cos^2 \theta_i \sin^2 \theta_j + \cos^2 \theta_j \sin^2 \theta_i)]$$

(You should check these are correct!) Then one solves the generalized eigenvalue problem,

$$\sum_j \mathcal{H}_{i,j} f_j = E \sum_j \mathcal{N}_{i,j} f_j. \quad (42)$$

To solve this, one has to construct

$$\mathbf{H} = \mathcal{N}^{-1/2} \mathcal{H} \mathcal{N}^{-1/2} \quad (43)$$

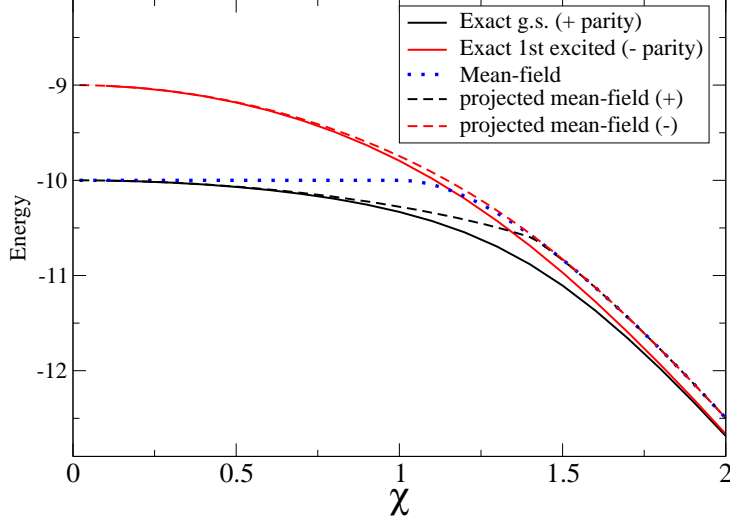


FIG. 3. Mean-field approximations to the Lipkin model with  $N = 20$ . Solid lines are the exact result from diagonalization of the ground state (black), which has positive parity, and the first excited state, which has negative parity. Dotted (blue) line is the unprojected mean-field solution. The dashed lines are variation after projection solutions, for the positive parity (black) and negative parity (red).

This can be tricky if the norm kernel is singular (has a zero eigenvalue) or near singular. The norm kernel should have non-negative eigenvalues, although due to roundoff error it could have slightly negative eigenvalues. Since most of the time we will have relatively small dimensions, this can be easily done by spectral decomposition: solve the eigenvalue problem for the norm kernel first, that is,

$$\sum_j \mathcal{N}_{ij} u_j^{(r)} = \nu^{(r)} u_j^{(r)}$$

where  $r$  labels the eigenpairs. Then one constructs

$$\left(\mathcal{N}^{-1/2}\right)_{ij} = \sum_{r, \nu^{(r)} > \epsilon} u_i^{(r)} \frac{1}{\sqrt{\nu^{(r)}}} u_j^{(r)} \quad (44)$$

where  $\epsilon$  is some cutoff for near-singular eigenvalues. The choice of  $\epsilon$  requires some experimentation and is the biggest fudge factor in these calculations. This may also haunt us later in applications to quantum computers, when we have noisy data, which will make near-singular norms more so.

By solving the generalized eigenvalue problem, that is, by finding the eigenpairs of (43) we will get excited states as well as the ground state. What is not immediately obvious, however, is if all these excited states belong to  $j_{\max} = \frac{N}{2}$  or some other  $j < j_{\max}$ .

### C. $\langle \hat{J}^2 \rangle$

We can test at least partially by computing

$$\langle \hat{J}^2 \rangle = \langle \hat{J}_z^2 + \hat{J}_x^2 + \hat{J}_y^2 \rangle = \langle \hat{J}_z^2 \rangle + \frac{1}{2} \langle \hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ \rangle.$$

Now

$$\langle \theta | \hat{J}_z^2 | \theta \rangle = N \langle 0 | \hat{c}(\theta) \hat{J}_z^2 \hat{c}^\dagger(\theta) | 0 \rangle + N(N-1) \langle 0 | \hat{c}(\theta) \hat{J}_z \hat{c}^\dagger(\theta) | 0 \rangle^2$$



$$= \frac{N}{4} (1 + (N-1) \cos^2 2\theta) = \frac{N}{4} (\sin^2 2\theta + N \cos^2 2\theta)$$

and

$$\begin{aligned} \langle \theta | \hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ | \theta \rangle &= N \langle 0 | \hat{c}(\theta) \left( \hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ \right) \hat{c}^\dagger(\theta) | 0 \rangle + 2N(N-1) \langle 0 | \hat{c}(\theta) \hat{J}_+ \hat{c}^\dagger(\theta) | 0 \rangle \langle 0 | \hat{c}(\theta) \hat{J}_- \hat{c}^\dagger(\theta) | 0 \rangle \\ &= N \left( 1 + \frac{1}{2} (N-1) \sin^2 2\theta \right). \end{aligned}$$

Adding these together,

$$\langle \hat{J}^2 \rangle = \langle \hat{J}_z^2 \rangle + \frac{1}{2} \langle \hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ \rangle = \frac{N}{2} + \frac{N^2}{4} = \frac{N}{4} (N+2) = \frac{N}{2} \left( \frac{N}{2} + 1 \right),$$

so the mean-field solution always belongs to  $j_{\max}$ . This makes sense, because for any  $\theta$ , there is an orientation at which we have maximal projection  $N/2$ .

#### D. Removing the (mostly) null space

As discussed above, we have to remove the subspace defined by eigenvalues in the norm kernel that are close to zero. This amounts to reducing the working dimension, that is, we must project from the dimension we are working in down to a smaller dimension. Hence, by modifying Eq. (44), we introduce the projection operator,

$$P_{ir} = \sum_{r, \nu^{(r)} > \epsilon} u_i^{(r)} \frac{1}{\sqrt{\nu^{(r)}}} \quad (45)$$

To do this, one should order the eigenvalues of  $\mathcal{N}$  from largest to smallest. That way, if one takes say  $n_\theta$  angles but the norm kernel has only  $n_{\text{ok}}$  eigenvalues  $\nu_r > \epsilon$ , with  $n_{\text{ok}} < n_\theta$ , then  $\mathcal{H}$  is  $n_\theta \times n_\theta$  square matrix, but  $\mathbf{P}$  is  $n_\theta \times n_{\text{ok}}$  rectangular matrix. Finally, one constructs  $\tilde{\mathbf{H}} = \mathbf{P}^\dagger \mathcal{H} \mathbf{P}$ , a square matrix of dimension  $n_{\text{ok}} \times n_{\text{ok}}$  and diagonalizes. If one need observables you will have to project back into the original space.

#### V. WORKING WITH MORE THAN ONE STATE

In what follows, I will modify the simple uniform approximation by including more than one state. Specifically, let's suppose generically we have states  $|x\rangle$  and  $|y\rangle$ , both of which are normalized. To carry out the calculation, we need the overlaps,

$$\langle x | y \rangle \quad (46)$$

and the off-diagonal matrix elements

$$\langle x | \hat{O} | y \rangle \quad (47)$$

In this, I follow Zhao et al. (arXiv:1902.10394) and introduce an ancillary qubit. Let

$$|\psi\rangle = \frac{1}{\sqrt{2}} [|0\rangle |x\rangle + |1\rangle |y\rangle] \quad (48)$$

Now apply the Hadamard gate to that first qubit

$$\mathbf{H}_1 |\psi\rangle = \frac{1}{2} [|0\rangle (|x\rangle + |y\rangle) + |1\rangle (|x\rangle - |y\rangle)] \quad (49)$$

Then the probability to measure 0 in the first qubit is

$$p_1(0) = \frac{1}{4} (\langle x|x\rangle + \langle x|y\rangle + \langle y|x\rangle + \langle y|y\rangle) = \frac{1}{2} (1 + \text{Re}\langle x|y\rangle) \quad (50)$$

or

$$\text{Re}\langle x|y\rangle = 2p_1(0) - 1 = p_1(0) - p_1(1). \quad (51)$$

To get the imaginary part, instead construct

$$|\psi\rangle = \frac{1}{\sqrt{2}} [|0\rangle|x\rangle - i|1\rangle|y\rangle] \quad (52)$$

and then

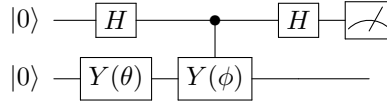
$$\text{Im}\langle x|y\rangle = 2p_1(0) - 1. \quad (53)$$

To measure a matrix element is similar.

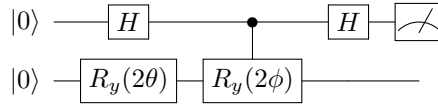
### A. Quantum circuit implementation

(Note: While I think the circuits are correct, the interpretation in terms of probabilities needs to be revisited.)

The generic circuit for the real part of the overlap is



or

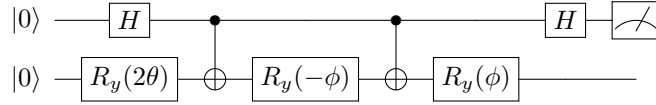


where the first qubit is the ancillary qubit. Then

$$\langle \theta | \theta + \phi \rangle_1 = p_1(0) - p_1(1). \quad (54)$$

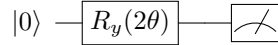
We expect this =  $\cos \phi$ . In our above assumptions we have only real values, so we do not need the imaginary part.

(Note: To implement a controlled rotation, if it is not part of Qiskit (?)



.)

To determine the matrix elements of  $\hat{J}_z$  we need to measure

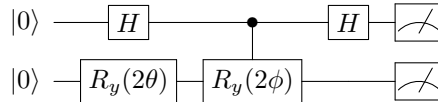


and evaluate

$$\langle \theta | \mathbf{Z} | \theta \rangle_1 = p(0) - p(1) \quad (55)$$

which we expect =  $\frac{1}{2} \cos 2\theta$ .

To get the off-diagonal matrix element of  $J_z$ , take



we have

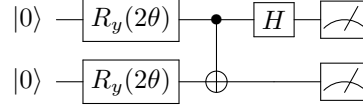
$$p_{12}(00) - p_{12}(01) = \frac{1}{4} [\langle \theta | \mathbf{Z} | \theta \rangle + \langle \theta + \phi | \mathbf{Z} | \theta + \phi \rangle + 2\langle \theta | \mathbf{Z} | \theta + \phi \rangle] \quad (56)$$

where  $p_{12}(ab)$  means to measure  $a$  in qubit 1 and  $b$  in qubit 2. I believe we can use more non-trivial information, and that

$$\langle \theta | \mathbf{Z} | \theta + \phi \rangle_1 = p_{12}(00) - p_{12}(01) - p_{12}(10) + p_{12}(11), \quad (57)$$

which we expect  $= \frac{1}{2} \cos(2\theta + \phi)$ .

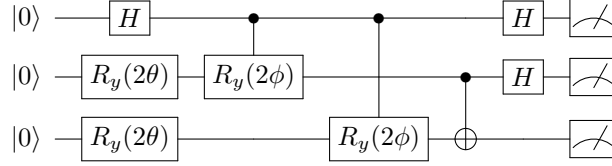
Finally, to measure the matrix element  $\hat{J}_+^2 + \hat{J}_-^2$ , let me repeat the diagonal



If we measure  $|00\rangle$ , then we were in the first Bell state with eigenvalue  $+1$ , and if we measure  $|10\rangle$  we were in second Bell state with eigenvalue  $-1$ . Therefore

$$\langle \theta | \hat{J}_+^2 + \hat{J}_-^2 | \theta \rangle_2 = p(00) - p(10) \quad (58)$$

which should  $= \frac{1}{2} \sin^2 2\theta$ , and the off-diagonal



I believe that

$$p_{123}(000) - p_{123}(010) = \frac{1}{4} \left[ \langle \theta | \hat{J}_+^2 + \hat{J}_-^2 | \theta \rangle_2 + \langle \theta + \phi | \hat{J}_+^2 + \hat{J}_-^2 | \theta + \phi \rangle_2 + 2 \langle \theta | \hat{J}_+^2 + \hat{J}_-^2 | \theta + \phi \rangle_2 \right]. \quad (59)$$

or,

$$\langle \theta | \hat{J}_+^2 + \hat{J}_-^2 | \theta + \phi \rangle_2 = p_{123}(000) - p_{123}(010) - p_{123}(100) + p_{123}(110), \quad (60)$$

which should  $= \cos^2 \theta \sin^2(\theta + \phi) + \cos^2(\theta + \phi) \sin^2 \theta$ .

This gives us all the matrix elements we need to solve the discretize Hill-Wheeler equation as in section IV B. The idea is to evaluate the elements of the kernels on a quantum computer and then solve the generalized eigenvalue problem classically.

Now let me explicitly express the matrix elements we need in terms of what we have circuits for:

$$\mathcal{N}(\theta, \theta') = \langle \theta | \theta' \rangle_N = (\langle \theta | \theta' \rangle_1)^N, \quad (61)$$

which  $= 1$  if  $\theta = \theta'$ , or use (54) otherwise; and

$$\begin{aligned} \mathcal{H}(\theta, \theta') &= -N\epsilon \langle \theta | \hat{J}_z | \theta' \rangle_1 (\langle \theta | \theta' \rangle_1)^{N-1} - \frac{V}{2} N(N-1) \langle \theta | \hat{J}_+^2 + \hat{J}_-^2 | \theta' \rangle_2 (\langle \theta | \theta' \rangle_1)^{N-2} \\ &= \left[ -N\epsilon \langle \theta | \hat{J}_z | \theta' \rangle_1 \langle \theta | \theta' \rangle_1 - \frac{V}{2} N(N-1) \langle \theta | \hat{J}_+^2 + \hat{J}_-^2 | \theta' \rangle_2 \right] (\langle \theta | \theta' \rangle_1)^{N-2} \end{aligned} \quad (62)$$

using (55) and (58) for  $\theta = \theta'$  and (57) and (60) for  $\theta \neq \theta'$ .

## VI. FUTURE WORK

We will generalize to a two-species Lipkin model with isospin, and then apply to a toy model of neutrinoless double-beta decay.

## VII. STEPS TOWARDS A PAPER

1. Numerically solve full Lipkin model, using matrix elements (7, 8).
2. Numerically solve variational approximation, using (20), and reproduce Fig. 2
3. Numerically find minimum of ‘parity-projected’ mean-field, (41), and add to Fig. 2.
4. Numerically solve generator coordinate equations and compare to excited states of full Lipkin solutions.
5. Implement quantum circuit(s) for mean-field Lipkin and simulate using Qiskit.

6. Implement quantum circuits for projected mean-field Lipkin and simulate using Qiskit.
7. Implement quantum circuits for generator coordinate Lipkin and simulate using Qiskit.