Prototyping many-body approximations in quantum computing

Calvin W. Johnson, and others, maybe

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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,

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

Here we write

$$\hat{J}_z = \frac{1}{2} \sum_{i=1}^{N} \hat{a}^\dagger_{i,\uparrow} \hat{a}_{i,\uparrow} - \hat{a}^\dagger_{i,\downarrow} \hat{a}_{i,\downarrow}, \tag{2}$$

$$\hat{J}_+ = \sum_i \hat{a}^\dagger_{i,\uparrow} \hat{a}_{i,\downarrow}, \tag{3}$$

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

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.

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: $|\Psi_T\rangle = \prod_{i=1}^N \hat{c}^\dagger_i |0\rangle$, Furthermore, I assume

$$\hat{c}^\dagger_i(\theta) = \hat{a}^\dagger_{i,\uparrow} \cos\theta + \hat{a}^\dagger_{i,\downarrow} \sin\theta, \tag{5}$$

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 θ is the same for all i, writing,

$$|\theta\rangle = \prod_{i=1}^{N} \hat{c}^\dagger_i(\theta) |0\rangle, \tag{6}$$

Note this is normalized, that is,

$$\langle \theta | \theta \rangle = \left(\langle 0 | \hat{c}(\theta) \hat{c}^\dagger(\theta) | 0 \rangle \right)^N = 1. \tag{7}$$

This makes evaluation easy. So for example,

$$\langle \hat{J}_z \rangle = \frac{1}{2} \sum_{i=1}^{N} \langle \theta | \hat{a}^\dagger_{i,\uparrow} \hat{a}_{i,\uparrow} - \hat{a}^\dagger_{i,\downarrow} \hat{a}_{i,\downarrow} | \theta \rangle \tag{8}$$

$$= \frac{1}{2} \sum_{i=1}^{N} \langle 0 | \hat{c}_i(\theta) \left(\hat{a}^\dagger_{i,\uparrow} \hat{a}_{i,\uparrow} - \hat{a}^\dagger_{i,\downarrow} \hat{a}_{i,\downarrow} \right) \hat{c}^\dagger_i(\theta) | 0 \rangle \tag{9}$$

$$= N \frac{1}{2} (\cos^2\theta - \sin^2\theta) = \frac{N}{2} \cos 2\theta \tag{10}$$

Similarly,

$$\langle\theta|\hat{J}_+^2 + \hat{J}_-^2|\theta\rangle = N(N-1)2\sin^2\theta\cos^2\theta = \frac{N(N-1)}{2}\sin^2 2\theta. \tag{11}$$

This means

$$\langle\hat{\mathcal{H}}\rangle = -\frac{N\epsilon}{2}\cos 2\theta - \frac{N(N-1)V}{4}\sin^2 2\theta = -\frac{N\epsilon}{2}\left[\cos 2\theta + \frac{(N-1)V}{2\epsilon}\sin^2 2\theta\right] \tag{12}$$

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

$$\frac{\partial}{\partial\theta}\langle\hat{\mathcal{H}}\rangle = -N\epsilon\left[-\sin 2\theta + \chi\sin 2\theta\cos 2\theta\right] = 0 \tag{13}$$

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.

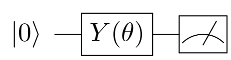
From this one can write analytically the "mean-field" approximation to the ground state energy:

$$E \approx \begin{cases} -\frac{N\epsilon}{2}, & \chi \leq 1; \\ -\frac{N\epsilon}{4}\left(\chi + \frac{1}{\chi}\right), & \chi \geq 1. \end{cases} \tag{14}$$

These of course agree at $\chi = 1$.

A. Implementation in a quantum circuit

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



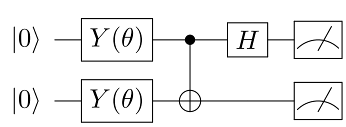
The $Y(\theta) = \exp(i\theta\mathbf{Y})$ gate rotates the qubit $|0\rangle = |\uparrow\rangle$ to $\cos\theta|0\rangle + \sin\theta|1\rangle$. The probability to measure in the $|0\rangle$ state is $\cos^2\theta$ while that to measure in the $|1\rangle$ state is $\sin^2\theta$, hence over many measurements

$$\langle\hat{J}_z\rangle = \frac{1}{2}\left(p(0) - p(1)\right) = p(0) - \frac{1}{2} = \frac{1}{2}\cos 2\theta. \tag{15}$$

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

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{16}$$

which has Bell states as eigenvectors: $\frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right)$ has eigenvalue 1, while $\frac{1}{\sqrt{2}}\left(|00\rangle - |11\rangle\right)$ 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

$$\langle\hat{J}_+^2 + \hat{J}_-^2\rangle = p(00) - p(10) = \frac{1}{2}\sin^2 2\theta \tag{17}$$

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

$$\frac{\left(\langle\theta| \pm \langle-\theta|\right)\hat{\mathcal{H}}\left(|\theta\rangle \pm |-\theta\rangle\right)}{\left(\langle\theta| \pm \langle-\theta|\right)\left(|\theta\rangle \pm |-\theta\rangle\right)} = \frac{\langle\theta|\hat{\mathcal{H}}|\theta\rangle \pm \langle-\theta|\hat{\mathcal{H}}|\theta\rangle}{1 \pm \langle-\theta|\theta\rangle}, \tag{18}$$

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,

$$\langle 0|\hat{c}_i(-\theta)\hat{c}^\dagger(+\theta)|0\rangle = \cos^2\theta - \sin^2\theta = \cos 2\theta, \tag{19}$$

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

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

$$\langle 0|\hat{c}(-\theta)\left(\hat{a}^\dagger_\uparrow\hat{a}_\uparrow - \hat{a}^\dagger_\downarrow\hat{a}_\downarrow\right)\hat{c}^\dagger(\theta)|0\rangle = \cos^2\theta + \sin^2\theta = +1, \tag{20}$$

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

$$\langle-\theta|\hat{J}_z|\theta\rangle = \frac{N}{2}\cos^{N-1}2\theta. \tag{21}$$

IV. GENERATOR COORDINATE

We can introduce a more general solution,

$$|\Psi\rangle = \int f(\theta')|\theta'\rangle\, d\theta'. \tag{22}$$

Then we get a generalized Schrödinger equation

$$\int f(\theta')\langle\theta|\hat{\mathcal{H}}|\theta'\rangle f(\theta')\, d\theta' = E\int f(\theta')\langle\theta|\theta'\rangle f(\theta')\, d\theta' \tag{23}$$

(In nuclear physics, the continuous parameter, here θ, is often associated with an observable, such as quadrupole deformation, that is treated as a generalized coordinate; furthermore one "generates" the state through a constrainted 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

$$\langle\theta|\theta'\rangle = \left(\cos\theta\cos\theta' + \sin\theta\sin\theta'\right)^N = \left(\cos(\theta-\theta')\right)^N, \tag{24}$$

and the elements of the Hamiltonian kernel, specifically,

$$\langle\theta|\hat{J}_z|\theta'\rangle = \frac{N}{2}\cos^{N-1}(\theta-\theta')\left(\cos\theta\cos\theta' - \sin\theta\sin\theta'\right) = \frac{N}{2}\cos^{N-1}(\theta-\theta')\cos(\theta+\theta'), \tag{25}$$

and

$$\langle\theta|\hat{J}^2_+ + \hat{J}^2_-|\theta'\rangle = N(N-1)\cos^{N-2}(\theta-\theta')\left(\cos^2\theta\sin^2\theta' + \cos^2\theta'\sin^2\theta\right). \tag{26}$$

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

$$\langle-\theta|\theta\rangle = \cos^N 2\theta, \tag{27}$$

$$\langle-\theta|\hat{J}_z|\theta\rangle = \frac{N}{2}\cos^{N-1}2\theta, \tag{28}$$

and

$$\langle -\theta|\hat{J}_+^2 + \hat{J}_-^2|\theta\rangle = N(N-1)\cos^{N-2}(2\theta)\frac{1}{2}\sin^2 2\theta. \tag{29}$$

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

$$E_\pm(\theta) = -\frac{N\epsilon}{2}\left[\cos 2\theta + \frac{(N-1)V}{2\epsilon}\sin^2 2\theta\right]\frac{1 \pm \cos^{N-2}(2\theta)}{1 \pm \cos^N(2\theta)}. \tag{30}$$

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

To solve the generator coordinate problem, one has to discretize the Hill-Wheeler integral and evaluate on a grid of θ, θ'. To be added.

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,

$$\langle x|y\rangle \tag{31}$$

and the off-diagonal matrix elements

$$\langle x|\hat{O}|y\rangle \tag{32}$$

In this, I follow Zhao et al. (arXiv:1902:10394) and introduce an ancillary qubit. Let

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left[|0\rangle|x\rangle + |1\rangle|y\rangle\right] \tag{33}$$

Now apply the Hadamard gate to that first qubit

$$\mathbf{H}_1|\psi\rangle = \frac{1}{2}\left[|0\rangle\left(|x\rangle + |y\rangle\right) + |1\rangle\left(|x\rangle - |y\rangle\right)\right] \tag{34}$$

Then the probability to measure 0 in the first qubit is

$$p_1(0) = \frac{1}{4}\left(\langle x|x\rangle + \langle x|y\rangle + \langle y|x\rangle + \langle y|y\rangle\right) = \frac{1}{2}\left(1 + \mathrm{Re}\langle x|y\rangle\right) \tag{35}$$

or

$$\mathrm{Re}\langle x|y\rangle = 2p_1(0) - 1. \tag{36}$$

To get the imaginary part, instead construct

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left[|0\rangle|x\rangle - i|1\rangle|y\rangle\right] \tag{37}$$

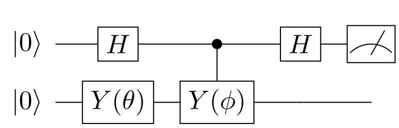
and then

$$\mathrm{Im}\langle x|y\rangle = 2p_1(0) - 1. \tag{38}$$

To measure a matrix element is similar.

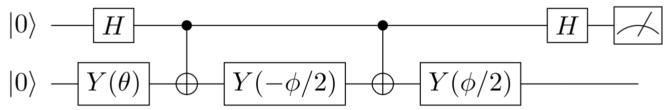
A. Quantum circuit implementation

The generic circuit for the real part of the overlap is

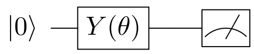


where the first qubit is the anciliary qubit. In our above assumptions we have only real values, so we do not need the imaginary part.

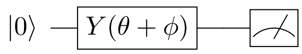
To implement a controlled rotation,



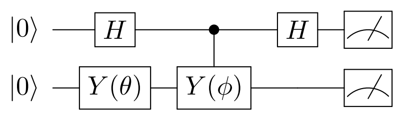
To determine the matrix elements of $\hat{J}_z$ we need to measure



to get $\langle\theta|\mathbf{Z}|\theta\rangle$,



to get $\langle\theta+\phi|\mathbf{Z}|\theta+\phi\rangle$, and finally,



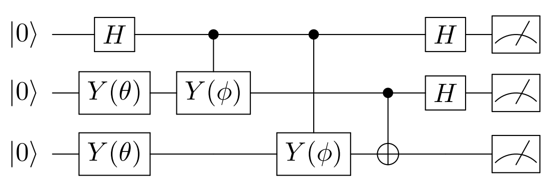
we have

$$p_{12}(00) - p_{12}(01) = \frac{1}{4}\left[\langle\theta|\mathbf{Z}|\theta\rangle + \langle\theta+\phi|\mathbf{Z}|\theta+\phi\rangle + 2\langle\theta|\mathbf{Z}|\theta+\phi\rangle\right] \tag{39}$$

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

$$p_{12}(00) - p_{12}(01) - p_{12}(10) + p_{12}(11) = \langle\theta|\mathbf{Z}|\theta+\phi\rangle. \tag{40}$$

Finally, to measure $\hat{J}_+^2 + \hat{J}_-^2$,



I believe that

$$p_{123}(000) - p_{123}(011) = \frac{1}{4}\left[\langle\theta|\hat{J}_+^2 + \hat{J}_-^2|\theta\rangle + \langle\theta+\phi|\hat{J}_+^2 + \hat{J}_-^2|\theta+\phi\rangle + 2\langle\theta|\hat{J}_+^2 + \hat{J}_-^2|\theta+\phi\rangle\right]. \tag{41}$$

or,

$$p_{123}(000) - p_{123}(011) - p_{123}(100) + p_{123}(111) = \langle\theta|\hat{J}_+^2 + \hat{J}_-^2|\theta+\phi\rangle. \tag{42}$$

This gives us all the matrix elements we need to solve the discretize Hill-Wheeler equation. (More on this soon.)