Investigation of the Nuclear Lipkin Model at Finite Temperature

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1 Introduction

Many nuclear systems of interest exist in high temperature environments, such as those found in heavy-ion collisions and stellar interiors, and therefore require the use of quantum statistical mechanics to determine relevant physical observables. However, determining the partition function of a quantum system, which is a necessary step for computing observables, requires knowledge of the entire spectrum of that system. While there exist a plethora of quantum many-body methods that are well-suited for studying nuclei, these methods are generally used to study the ground state and low-lying excited states. In nuclei the number of excited states grows exponentially with excitation energy [1], leading to complex spectra that are ill-suited for studying using these methods. Therefore, rather than attempt to calculate the complete nuclear spectrum directly, we can instead seek finite-temperature methods that can be used to calculate thermal averages of observables directly.

1.1 Project Overview

Here we test such a method, the finite-temperature Hartree-Fock (HF) approximation, by applying it to a solvable model known as the Lipkin model [2]. The Hamiltonian of the Lipkin model can be expressed in terms of an SU(2) algebra and therefore has a block diagonal structure, corresponding to the various SU(2) representations, that can diagonalized directly to obtain the full spectrum (and thus exact thermal averages) of the model. The main quantities we are interested in are the thermal energy E (which we will occasionally refer to as simply the energy), which we know should reduce to the Lipkin model ground state energy in the $T \to 0$ limit, and the free energy F, which is necessary for analyzing phase transitions.

2 Finite-Temperature Hartree-Fock Method

First we will discuss the finite temperature Hartree-Fock (HF) approximation. Consider a Hamiltonian that contains a single-particle part and a two-body interaction

$$H = \sum_{i,j} t_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \tag{1}$$

In order to calculate thermodynamic observables, we need to determine the system's density matrix. For a given temperature T and chemical potential μ (we choose μ rather than N due to the theory of fermionic systems at finite temperature being more tractable when N is allowed to vary), the density matrix of the equilibrium state is given by

$$\hat{D} = \frac{1}{Z} e^{-\beta \hat{H} - \alpha \hat{N}} \tag{2}$$

where (in units such that $k_B = 1$) $\beta = 1/T$, $\alpha = -\mu\beta$ and

$$Z = \mathrm{Tr}(\hat{D}) = \mathrm{Tr}(e^{-\beta \hat{H} - \alpha \hat{N}}) \tag{3}$$

is the partition function that ensures $\hat{D}$ is normalized. We know that this density matrix minimizes the grand potential of the system, which is given by

$$\Omega(\hat{D}) = E - TS - \mu N \tag{4}$$

where

$$E = \mathrm{Tr}(\hat{D}\hat{H}) \tag{5}$$

$$S = -\mathrm{Tr}(\hat{D}\ln\hat{D}) \tag{6}$$

$$N = \mathrm{Tr}(\hat{D}\hat{N}) \tag{7}$$

Thus far, everything has been exact, and if we knew the spectrum of H then the problem would be solved, as any observable of interest can be computed using $\langle\hat{O}\rangle = \mathrm{Tr}(\hat{D}\hat{O})$. However, for most systems of interest obtaining the full spectrum is computationally intractable, thus we require an approximation scheme. To do so, let us emulate the zero-temperature HF method by replacing the full Hamiltonian in the density matrix with a one-body Hamiltonian describing a non-interacting system, which gives a density matrix

$$\hat{D}_{\mathrm{HF}} = e^{-\beta\hat{K}-\alpha\hat{N}} \tag{8}$$

where $\hat{K} = \sum k_{ij}a_i^\dagger a_j$. With this assumption, if we further define the single particle density as

$$\rho_{ij} = \mathrm{Tr}(\hat{D}_{\mathrm{HF}}a_j^\dagger a_i) = \left(\frac{1}{1+e^{\beta\hat{K}+\alpha}}\right)_{ij} \tag{9}$$

where the second equality is the well-known form of the single particle density for non-interacting fermions, then it can be shown that

$$E = \mathrm{tr}(t\rho) + \frac{1}{2}\mathrm{tr}(\Gamma\rho) \tag{10}$$

$$S = -\mathrm{tr}(\rho\log\rho) - \mathrm{tr}[(1-\rho)\log(1-\rho)] \tag{11}$$

$$N = \mathrm{tr}(\rho) \tag{12}$$

where t is the matrix with components t_{ij}, $\Gamma_{ij} = \sum_{k,l}(v_{ikjl} - v_{iklj})\rho_{lk} = \sum_{k,l}\overline{v}_{ikjl}\rho_{lk}$, and tr denotes a trace over the single particle states. Now, Eq. 10 holds for arbitrary $\hat{K}$. However, just as in the zero-temperature HF approximation, we seek the $\hat{K}$ that minimizes the relevant energy of our system–here, the grand potential given by Eq. 4. One can show that the operator $\hat{K}$ that minimizes Eq. 4 is

$$\hat{K} = t + \Gamma \equiv h[\rho] \tag{13}$$

which, just as in HF, we refer to as the mean-field Hamiltonian.

In theory, given h we can obtain the thermal energy of the system through Eq. 10, taking ρ as given in Eq. 9 with $\hat{K} = h$. However, we can see that h itself depeneds on ρ, meaning, just as in HF, we have a self-consistency equation that must be solved numerically, namely

$$\rho = \frac{1}{1+e^{\beta h[\rho]+\alpha}} \tag{14}$$

One way to solve this is to convert it into an eigenvalue equation. To do so, note that the eigenbasis of h, which we'll denote as $c_k^\dagger$, is related to $a_l^\dagger$, the basis that our Hamiltonian is written with respect to, by a unitary transformation D that satisfies

$$c_k^\dagger = \sum_l D_{lk}a_l^\dagger \tag{15}$$

which means that the matrix elements of ρ in the $a_l^\dagger$-basis are

$$\rho_{ll'} = \sum_{k,k'} D_{lk}D^*_{l'k'}\rho_{kk'} \tag{16}$$

Of course, by Eq. 14 we see that in the eigenbasis of h

$$\rho_{kk'} = \delta_{kk'}\frac{1}{1+e^{\beta\epsilon_k+\alpha}} \equiv \delta_{kk'}f_k \tag{17}$$

where ϵ_k is the k_{th} eigenvalue of h. We refer to the function f_k as the k_{th} occupation number. We then have

$$\rho_{ll'} = \sum_k D_{lk}D^*_{l'k}f_k \tag{18}$$

Of course, in the $a_l^\dagger$ basis we know that D_{lk} are the elements of the vector representing the eigenbasis $c_k^\dagger$, which tells us, for a given k, that we further require

$$\sum_{l'} h_{ll'} D_{l'k} = \epsilon_k D_{lk} \tag{19}$$

Using Eq. 13 to replace h and inserting Eq. 18 into the definition of Γ, we finally arrive at the set of finite-temperature Hartree-Fock eigenvalue equations for a given k, namely

$$\sum_{l'} \left[t_{ll'} + \sum_{pp'} \overline{v}_{lp'l'p} \left(\sum_i D_{pi} D^*_{p'i} f_i \right) \right] D_{l'k} = \epsilon_k D_{lk} \tag{20}$$

These equations can be solved iteratively for the matrix elements D_{lk} and the single particle energies ϵ_k to determine ρ using Eq. 18, from which we can calculate the thermal HF energy, E, via Eq. 10

3 The Nuclear Lipkin Model

3.1 General Formalism

The Lipkin model of the nucleus is a simple model of N nucleons occupying two levels with energies $-\epsilon/2$ and $\epsilon/2$, each of angular momentum j so that we have a maximum level degeneracy of $2j+1$. We further assume that there are two-body interactions of strength V between nucleons in the upper level and nucleons in the lower level. For simplicity we assume that the shell is full, i.e. $N = 2j+1$. If we let $a_m^\dagger$ correspond to a state in the upper level for $m > 0$ and in the lower level for $m < 0$, then we can write the Hamiltonian describing this system as

$$H = \frac{\epsilon}{2} \sum_{m>0}^{N} \left(a_m^\dagger a_m - a_{-m}^\dagger a_{-m} \right) - \frac{V}{2} \sum_{m,m'>0}^{N} \left(a_m^\dagger a_{-m} a_{m'}^\dagger a_{-m'} + a_{-m}^\dagger a_m a_{-m'}^\dagger a_{m'} \right) \tag{21}$$

If we define the operators

$$K_0 = \frac{1}{2} \sum_{m>0}^{N} \left(a_m^\dagger a_m - a_{-m}^\dagger a_{-m} \right) \tag{22}$$

$$K_+ = \sum_{m>0}^{N} a_m^\dagger a_{-m} = (K_-)^\dagger \tag{23}$$

then Eq. 21 becomes

$$H = \epsilon K_0 - \frac{1}{2} V \left(K_+^2 + K_-^2 \right) \tag{24}$$

It can be easily showed that these operators form an $SU(2)$ algebra, i.e.

$$[K_0, K_\pm] = \pm K_\pm \tag{25}$$

$$[K_+, K_-] = 2K_0 \tag{26}$$

prompting us to refer to these as "quasi-spin" operators. In the quasi-spin basis $|kk_0\rangle$ we have

$$\begin{aligned} \langle kk_0|H|kk_0'\rangle = \epsilon k_0 \delta_{k_0,k_0'} - \frac{1}{2} V \Bigg(& \sqrt{(k-k_0)(k+k_0+1)(k+k_0')(k-k_0'+1)}\, \delta_{k_0'-1,k_0+1} \\ & + \sqrt{(k+k_0)(k-k_0+1)(k-k_0')(k+k_0'+1)}\, \delta_{k_0'-1,k_0+1} \Bigg) \end{aligned} \tag{27}$$

For a given k (where $k \in \{0, 1, ..., N/2\}$ for N even and $k \in \{1/2, 3/2, ..., N/2\}$ for N odd) we can solve the $(2k+1) \times (2k+1)$ matrix formed from Eq. 27 to find the energy eigenvalues $E_{k,i}$ of H within that $k-$subspace, which can then be used to compute the canonical partition function of that subspace as

$$\zeta_k = \sum_i e^{-E_{k,i}\beta} \tag{28}$$

The degeneracy of a given k subspace for a N nucleon system is given by, as is seen in Ref. [3],

$$g_k = \frac{N!^2}{(N/2-k)!^2(N/2+k)!^2} - \frac{N!^2}{(N/2-k-1)!^2(N/2+k+1)!^2} \tag{29}$$

which makes the full canonical partition function of the system

$$Z = \sum_{k=0,1/2}^{N/2} g_k \zeta_k \tag{30}$$

$$= \sum_{k=0,1/2}^{N/2} \left[\left(\frac{N!^2}{(N/2-k)!^2(N/2+k)!^2} - \frac{N!^2}{(N/2-k-1)!^2(N/2+k+1)!^2} \right) \sum_i e^{-E_{k,i}\beta} \right] \tag{31}$$

We can thus calculate (numerically) the exact energy of the system at a given T as

$$E = \frac{1}{Z} \sum_{k=0,1/2}^{N/2} \left(g_k \sum_i E_{k,i} e^{-E_{k,i}\beta} \right) \tag{32}$$

This equation will be used to test the accuracy of the finite-temperature HF method described in Section 2 .

3.2 Hartree-Fock Approximation

To apply Eq. 20 to the Lipkin model Hamiltonian 21, let us make the simplifying assumption that only states with the same $|m|$ are mixed by the matrix D – that is, we have the transformed states being $c^\dagger_{0m}, c^\dagger_{1m}$ for each m, defined by

$$\begin{pmatrix} c^\dagger_{0m} \\ c^\dagger_{1m} \end{pmatrix} = \begin{pmatrix} D_{-0} & D_{+0} \\ D_{-1} & D_{+1} \end{pmatrix} \begin{pmatrix} a^\dagger_{-m} \\ a^\dagger_m \end{pmatrix} \tag{33}$$

where the matrix elements are independent of the value of m. This tells us that there will only be two unique eigenvalues of the matrix h, which we call $\epsilon_{0,1}$ and the associated occupation numbers we call $f_{0,1}$. With this, one can show that Eq. 20 can be expressed as

$$\begin{pmatrix} -\epsilon/2 & -V\left(D_{+0}D^*_{-0}f_0 + D_{+1}D^*_{-1}f_1\right)(N-1) \\ -V\left(D_{-0}D^*_{+0}f_0 + D_{-1}D^*_{+1}f_1\right)(N-1) & \epsilon/2 \end{pmatrix} \begin{pmatrix} D_{-0,-1} \\ D_{+0,+1} \end{pmatrix} = \epsilon_{0,1} \begin{pmatrix} D_{-0,-1} \\ D_{+0,+1} \end{pmatrix} \tag{34}$$

This equation can be solved numerically using an iterative method for the matrix elements D and subsequently plugged into Eq. 10 to obtain the HF energy of the system, which under these assumptions can be shown to be equal to

$$E = -\frac{N\epsilon}{2} \left[\left(|D_{-0}|^2 - |D_{+0}|^2 \right) f_0 + \left(|D_{-1}|^2 - |D_{+1}|^2 \right) f_1 \right. \tag{35}$$
$$\left. + \chi \left(\left(D_{+0}D^*_{-0}f_0 + D_{+1}D^*_{-1}f_1 \right)^2 + \left(D_{-0}D^*_{+0}f_0 + D_{-1}D^*_{+1}f_1 \right)^2 \right) \right]$$

where $\chi = V(N-1)/\epsilon$.

If we assume that D is a real matrix then we know that, since it's orthogonal, its components can be written in the form $D_{-0} = \cos\alpha = D_{+1}, D_{+0} = \sin\alpha = -D_{-1}$ for some angle α. In this case, Eq. 35 becomes

$$E(\alpha) = -\frac{N\epsilon}{2} \left[\left(\cos^2\alpha - \sin^2\alpha \right) f_0 + \left(\cos^2\alpha - \sin^2\alpha \right) f_1 + 2\chi \left(f_0 \sin\alpha\cos\alpha - f_1 \cos\alpha \sin\alpha \right)^2 \right] \tag{36}$$

This form will be useful for analyzing phase transitions of the model, which we do in Sec. 3.2.1

3.2.1 Phase Transitions

The thermal energy E isn't our only quantity of interest–we are also interested in determining whether any thermal phase transitions exist. It is well known that the zero temperature HF approximation of the Lipkin model has a second-order quantum phase transition with respect to α when $\chi = 1$, as found in Ref. [4]. As the chemical potential of the Lipkin model is 0 when $N = 2j+1$ (which can be easily seen from the condition that $f_0 + f_1 = 1$ in a full shell), we can identify thermal phase transitions by studying the free energy

$$F = E - TS \tag{37}$$

as a function of the order parameter α and identifying its critical points as we vary T. Using $E(\alpha)$ from Eq. 36 and

$$S = -2N\left(f_0 \ln f_0 + f_1 \ln f1\right) \tag{38}$$

we find $F(\alpha)$ at a given T, N, χ to be

$$\begin{aligned} F(\alpha) =& 2NT\left(f_0 \ln f_0 + f_1 \ln f1\right) \\ &- \frac{N\epsilon}{2}\left[\left(\cos^2\alpha - \sin^2\alpha\right) f_0 + \left(\cos^2\alpha - \sin^2\alpha\right) f_1 + 2\chi\left(f_0 \sin\alpha\cos\alpha - f_1 \cos\alpha \sin\alpha\right)^2\right] \end{aligned} \tag{39}$$

It should be noted that the occupation numbers $f_{0,1}$ depend non-trivially on α. This is evident from Eq. 34 in which we see that the HF energies $\epsilon_{0,1}$ depend on the matrix elements D, and thus α. As $f_{0,1}$ are functions of $\epsilon_{0,1}$ we must first solve, for fixed α (and thus fixed elements D), the HF equations 34 for $\epsilon_{0,1}$ in order to compute the occupation numbers. However, due to the structure of Eq. 34 we can see that ϵ_0 satisfies the self-consistency equation

$$\epsilon_0 = -\epsilon\left(\frac{1}{4} + \frac{V}{\epsilon}(N-1)\left[(f_0 \sin\alpha\cos\alpha)^2 + (f_1 \sin\alpha\cos\alpha)^2 - 2f_0 f_1 \cos\alpha^2 \sin\alpha^2\right]\right)^{1/2} = -\epsilon_1 \tag{40}$$

Thus, for each α we can numerically solve this equation for $\epsilon_{0,1}$ to obtain the occupation numbers so that we can then compute F in accordance with Eq. 39.

4 Results

The solution to Eq. 34 for the matrix elements $D_{\pm 0}, D_{\pm 1}$ was carried out using the `numpy` package in Python. The same python script was also used to calculate the exact energy of the system in accordance with Eq. 32. The results of both calculations for $0 \leq T \leq 20$ using $N = 10, \epsilon = 0.5$, and $V = 0.1$ can be found in Fig. 1. We further performed a zero-temperature analysis of the Lipkin model, both exactly and via the zero-temperature HF method, to ensure that we recovered the correct limiting behavior of the finite-temperature energies as $T \to 0$. These calculations can also been seen in Fig. 1, depicted as open circles located at $T = 0$.

The free energy as a function of alpha, given by Eq. 39, for $\chi = 1.8$ and $\chi = 0.9$ is shown in Fig. 2. These values of χ were chosen as at $T = 0$ these correspond to the two different quantum phases of the HF approximation of the Lipkin model: a minimum at $\alpha = 0$ for $\chi = 0.9$ and a minimum at $\alpha \neq 0$ at $\chi = 1.8$, with the quantum phase transition occurring at $\chi = 1$. From Fig. 3 we can see that only systems in the $\chi > 1$ quantum phase can undergo a thermal phase transition. To determine the order of the phase transition we calculated the heat capacity C of the HF approximation of $E(T)$, Eq. 35 (where both the occupation numbers $f_{0,1}$ and the matrix elements D are functions of T), which was done by computing the numerical derivative $C = \partial E/\partial T$ using central differencing. This was then compared to the exact heat capacity of the Lipkin model, which was computed from the partition function, Eq. 30, using $C = \left(\langle E^2\rangle - \langle E\rangle^2\right)/T^2$. The results are displayed in Fig. 4. Further information useful for analyzing the phase transition behavior is plotting the equilibrium value of α (i.e., the value of α that minimizes $F(\alpha)$) as a function of T. For a second order transition we expect $\alpha_{min}(T)$ to vary continuously. This information is presented in Fig. 5.

5 Conclusion

5.1 Discussion

We can see from Fig. 1 that the finite-temperature Hartree-Fock approximation we discussed in Sec. 2 is in good agreement with the exact energy, especially at high temperatures. Using the built-in `time` Unix command, we see that our HF code takes, on average, 0.4 seconds to compute the energy for 200 values of T, whereas the code calculating the exact solution took an average of 0.55 seconds. Further, the CPU usage was significantly lower, on average, for the HF code. Therefore, the HF method provides a computationally inexpensive way to obtain accurate measurements of the internal energy of the nuclear Lipkin model at finite temperature. We could improve the accuracy further by involving mixing of states with different values of $|m|$, at the cost of increased computational complexity.

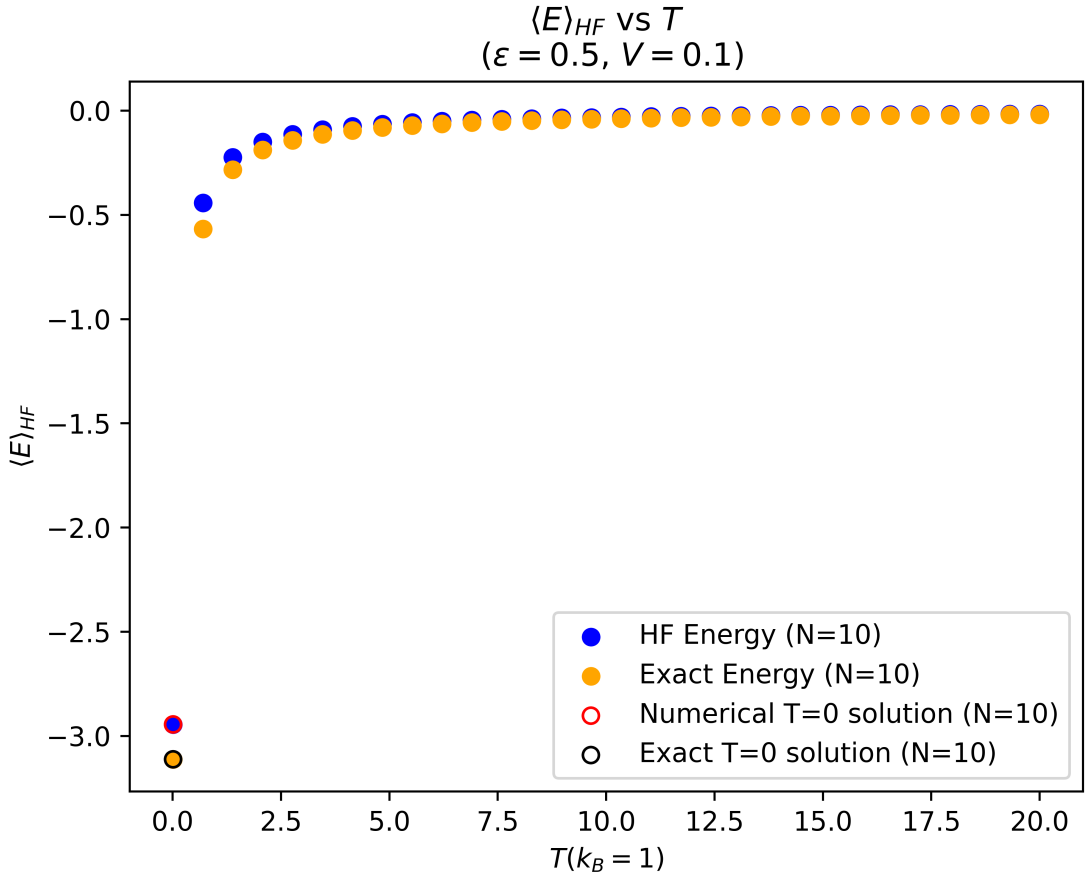


Figure 1: The HF approximation of the thermal energy as a function of T, calculated using Eq. 35, is displayed as blue circles. For comparative purposes we also have the exact energy as a function of T, shown by orange circles. We have chosen a system such that $N = 10$, $\epsilon = 0.5$ and the interaction strength is $V = 0.1$, in units such that $k_B = 1$. We can see that the HF approximation provides a good approximation of the exact energy, with the two converging in the high T limit. The results of the T=0 calculations are shown by open circles: a black circle for the exact ground-state energy and a red circle for the T=0 HF energy.

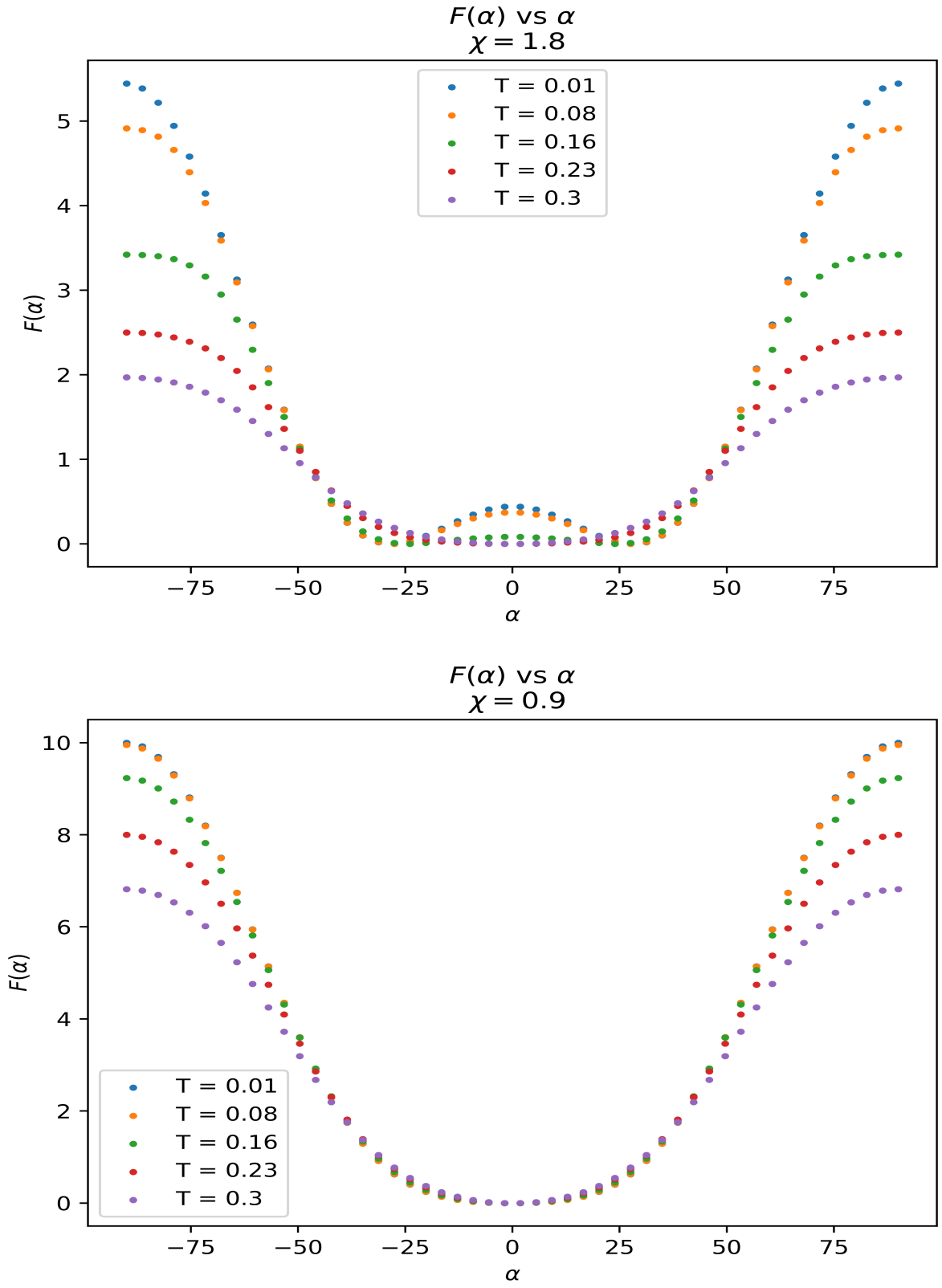


Figure 2: The free energy $F(\alpha)$ plotted as a function of α, given by Eq. 39. The top panel is for $\chi = 1.8$, which we can see undergoes a thermal phase transition at $T \approx 0.2$, while the bottom panel corresponds to $\chi = 0.9$, for which no thermal phase transition occurs.

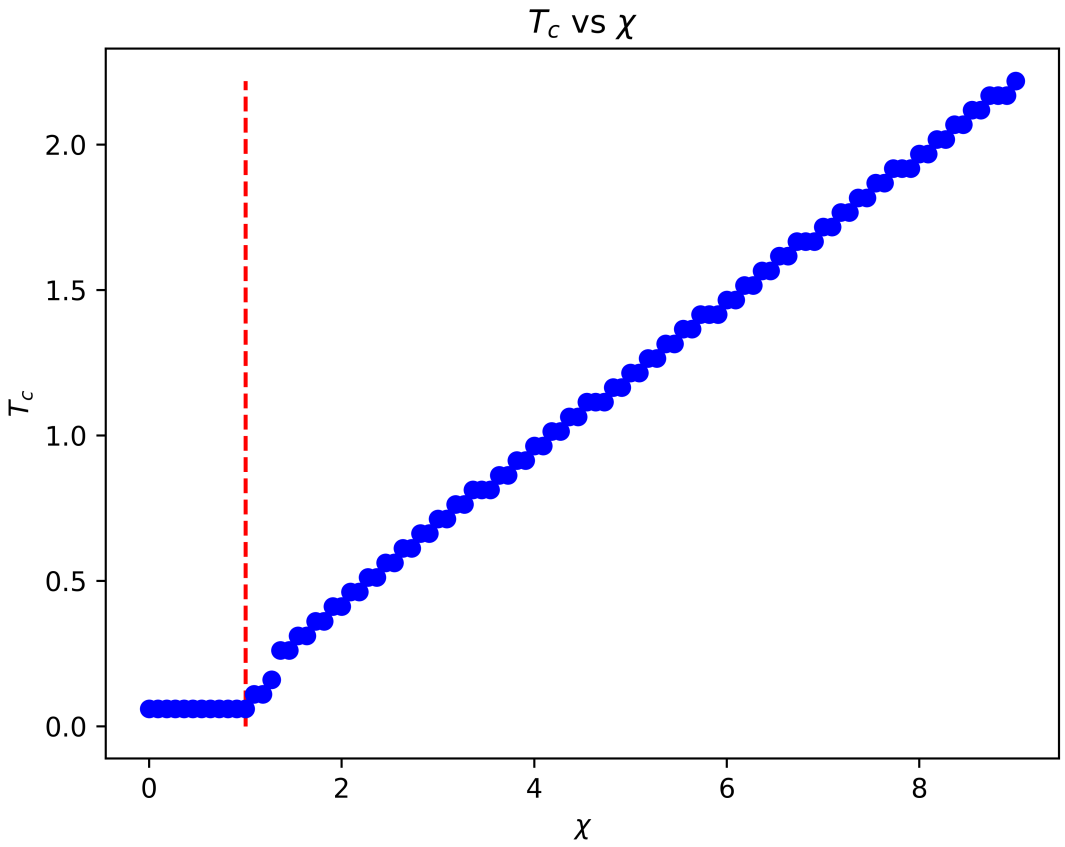
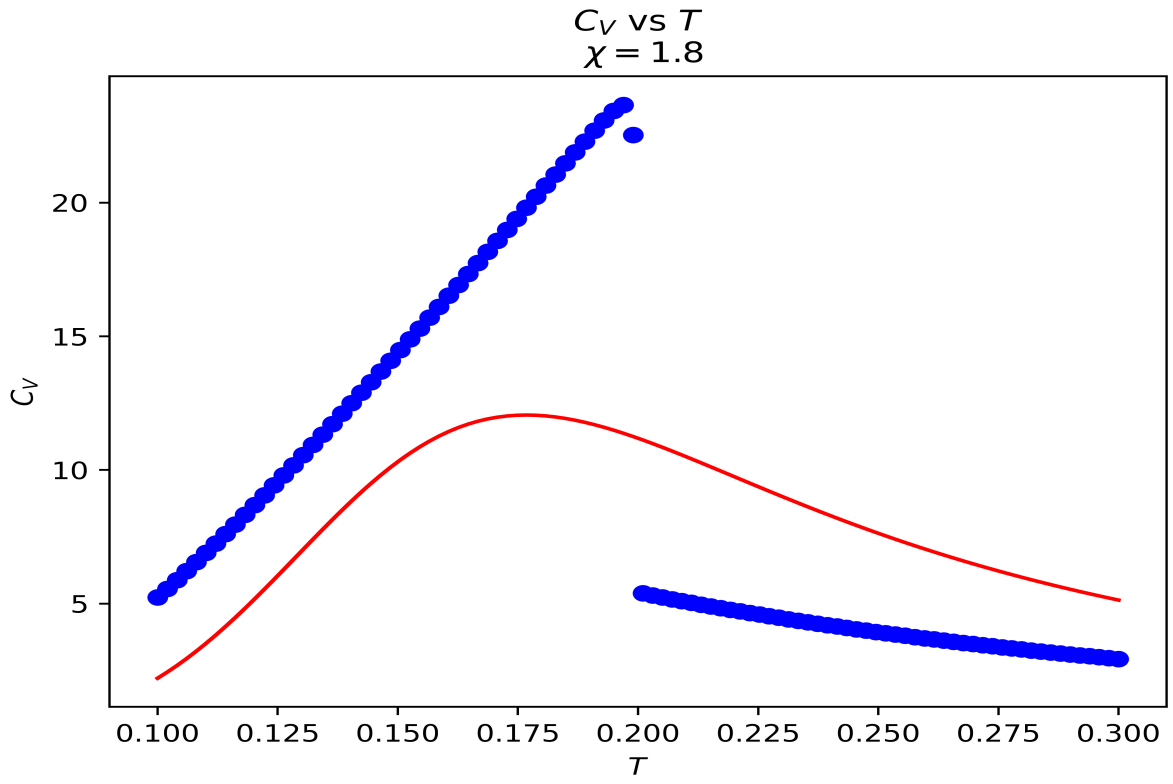
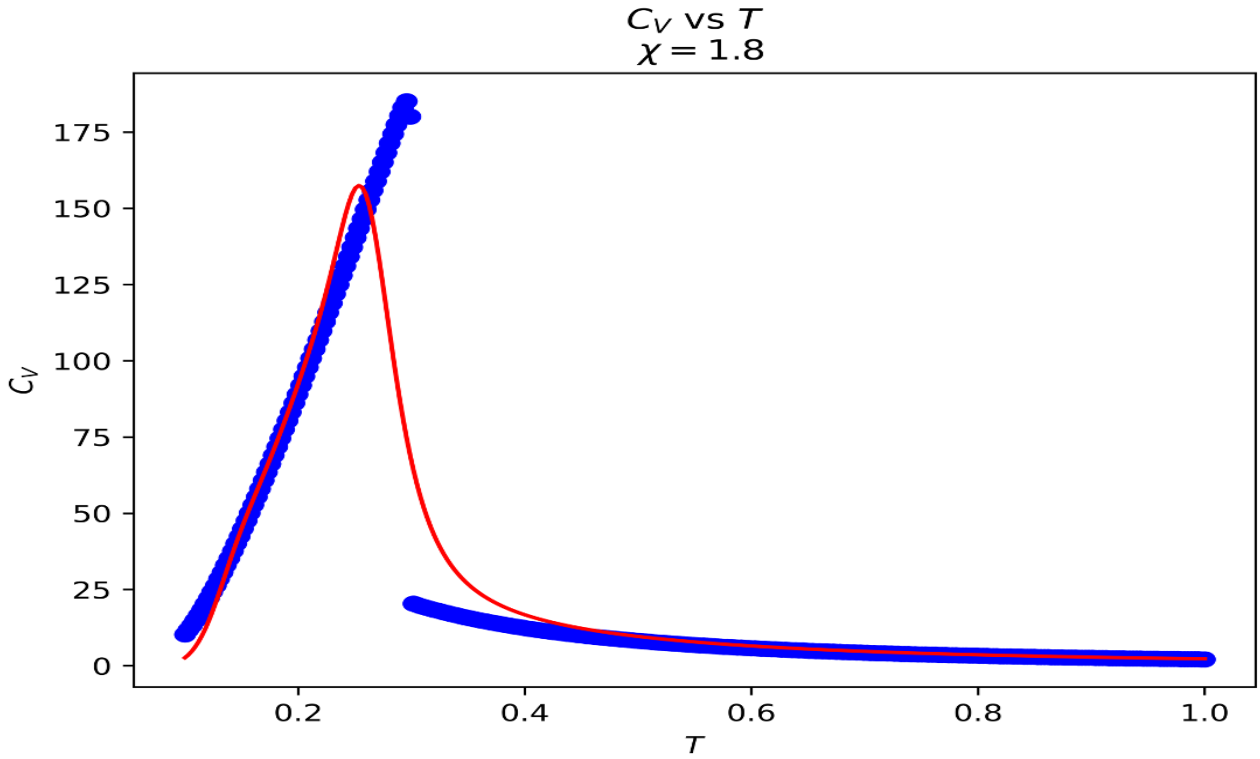


Figure 3: The critical temperature T_c as a function of the parameter χ. We see no phase transition occurs for $\chi < 1$, as expected, while T_c increases linearly with χ for $\chi > 1$



(a) The heat capacity for $N = 10$. We see the exact solution is smooth and deviates significantly from the HF approximation



(b) The heat capacity for $N = 70$. We see the exact solution is a much closer match in structure to the HF approximation, indicating that the exact solution exhibits a phase transition in the thermodynamic limit

Figure 4: The heat capacity of the Lipkin model, calculated numerically using the HF thermal energy $E(T)$, is displayed as blue dots for $\chi = 1.8$. The top panel corresponds to $N = 10$ whereas the bottom panel is $N = 70$. We can see a clear discontinuity at $T \approx 0.2$, indicating a thermal phase transition at this critical temperature. The red line corresponds to the exact heat capacity, which exhibits no discontinuity.

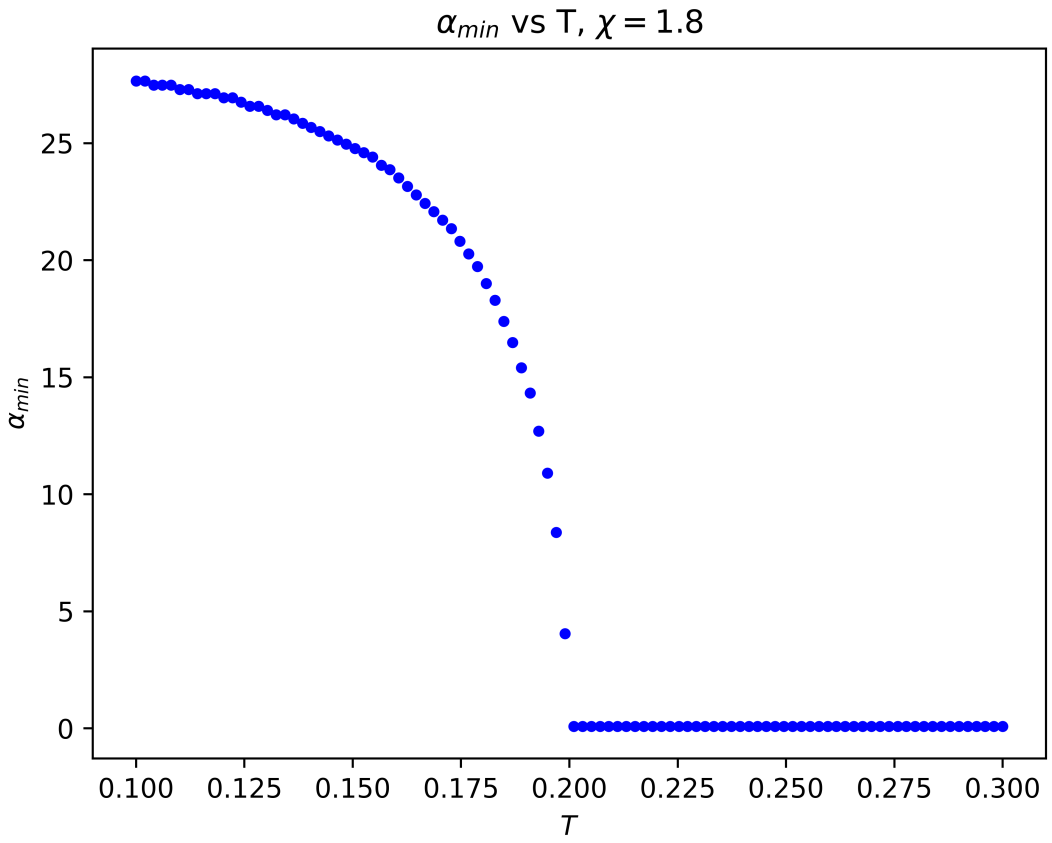


Figure 5: The equilibrium value of the order parameter α as a function of T for $\chi = 1.8$. We can see that α varies continuously at the critical temperature $T \approx 0.2$, indicating a phase transition of second order.

Furthermore, we observe from the top panel of Fig. 2 that, in the HF mean-field approximation, the $\chi > 1$ regime undergoes a thermal phase transition to the $\alpha_{eq} = 0$ phase (corresponding to the $\chi < 1$ quantum phase) at some critical temperature T_c (in Fig. 2 we have $T_c \approx 0.2$). From the bottom panel of Fig. 2 we see that no such thermal phase transition occurs for $\chi < 1$. We can further see that this transition is second-order; this is made evident by the fact that α_{min} varies continuously with respect to T, as seen in Fig. 5, and that there is a discontinuity in the heat capacity, as depicted in Fig. 4. We note that the exact heat capacity of the Lipkin model, which can be found in Fig. 4, shows no phase transition, as it varies smoothly with respect to T. This indicates that the transition is solely an artifact of our approximation scheme, confirming that, strictly speaking, no phase transition can occur in a finite-size system [5]. We do note that, by comparing Fig. 4a to Fig. 4b, we expect a phase transition to occur in the thermodynamic limit of the exact solution.

5.2 Concluding Thoughts

This project was performed to get myself familiar with the methods and concepts utilized in Dr. Alhassid's group. In more realistic nuclear systems, it is necessary to include the effects of correlations beyond the mean-field approximation. Nevertheless, the mean-field approximation is often a first step in the study of more complicated quantum many-body systems. My goals for this project didn't vary much over the course of the semester, as I was able to carry out the full derivation of the finite-temperature HF equations both generally (Eq. 20) and for the Lipkin model (Eq. 34) and numerically implement them to solve for the thermal energy. One variation did occur, however, which was the phase transition analysis. Initially I didn't suspect to have sufficient time to perform such an analysis within the semester time-frame, but I ended up having ample time to do so.

Moving forward, I will begin using more sophisticated finite temperature methods to study more complicated nuclear models.

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