The Lipkin model at finite temperature

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Abstract: We consider a system of N fermions described by the Lipkin model and investigate their behaviour at finite temperature. We study the influence of the interactions on thermodynamic properties. The calculations have been done by a numerical diagonalization of the Hamiltonian. Once the full spectrum is known we consider the thermal occupation of the states and calculate the different thermodynamic properties. The extension of the Hellmann-Feynman theorem at finite temperature requires the derivative of the free energy instead of the internal energy used for zero temperature. The importance of the entropy in the fulfillment of the Hellmann-Feynman theorem is analyzed.

I. INTRODUCTION

Solving the Schrödinger equation for a many-body system has supposed a challenge for physicists along the history. These difficulties in solving this equation have induced the development and improvement of quantum many-body theories. Simple model systems have been proposed in order to obtain exact solutions. One of these models is the Lipkin model. It was proposed in the mid-60s by Lipkin, Meshkov and Glick[1] to describe a many-fermion system with two energy levels. It is important to highlight that the Lipkin model can provide exact results and has been set as a benchmark for different approximations as for instance Hartree-Fock, random phase approximation and perturbation theory[2, 3] and also to study quantum phase transitions[4] and protocols to implement short-cuts to adiabaticity[5, 6].

The aim of this work is the study of this model at finite temperature. The motivation arises from the interest to study hot nuclei and hot nuclear matter in heavy ion collisions and in supernova explosions. Theoretical treatments of these issues require of finite temperature many-body theory. The Lipkin model has been widely used at zero temperature but not as much at finite temperature[7–9].

The organization of this work is as follows. In Sec. II the basis of the Lipkin model are explained. In Sec. III we make a detailed study of the Lipkin model at finite temperature (with and without interaction). In Sec. IV we prove the validity of the Hellmann-Feynman theorem at finite temperature. Finally, a short summary of our results is contained in Sec. V.

II. THE LIPKIN MODEL

The Lipkin model consists of N fermions occupying two energy levels. The energy difference between these two levels is indicated with the letter ϵ. Each level is described by a quantum number σ which takes the value +1 in the upper level and -1 in the lower one. It is also characterized by a set of p quantum numbers specifying the site number $(1, ..., N)$. The Hamiltonian of this model is given by:

$$\hat{H} = \epsilon \hat{K}_0 - \frac{V}{2}(\hat{K}_+^2 + \hat{K}_-^2), \tag{1}$$

with

$$\begin{aligned} \hat{K}_0 &= \frac{1}{2}\sum_{p=1}^{N}(a_{p,+}^\dagger a_{p,+} - a_{p,-}^\dagger a_{p,-}), \\ \hat{K}_+ &= \sum_{p=1}^{N} a_{p,+}^\dagger a_{p,-}, \\ \hat{K}_- &= \sum_{p=1}^{N} a_{p,-}^\dagger a_{p,+}, \end{aligned} \tag{2}$$

where $a_{p,\pm}^\dagger$, $a_{p,\pm}$ are the creation and annihilation operators satisfying the anti-commutation relations:

$$\{a_{p,\alpha}, a_{r,\beta}^\dagger\} = \delta_{pr}\delta_{\alpha\beta}. \tag{3}$$

In the Hamiltonian that we are considering, the term proportional to V is the interaction term and acts as follows: it takes two particles from one level and puts them on the other one. Therefore, without interaction we would only have the term $\hat{K}_0$. The energies in this unperturbed situation are given by the number of particles lying in the lower and upper levels. The new operators that we have introduced satisfy the following commutation relations characteristic of the algebra of angular momentum:

$$[\hat{K}_+, \hat{K}_-] = 2\hat{K}_0, [\hat{K}_0, \hat{K}_+] = \hat{K}_+, [\hat{K}_0, \hat{K}_-] = -\hat{K}_-, \tag{4}$$

which can be easily proved using the anti-commutation relations in Eq. (3). The action of these operators is

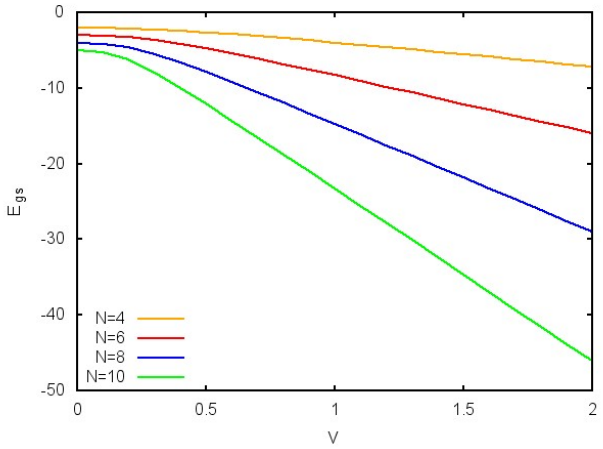

FIG. 1: Evolution of the ground state energy versus the interaction term V for different number of particles.

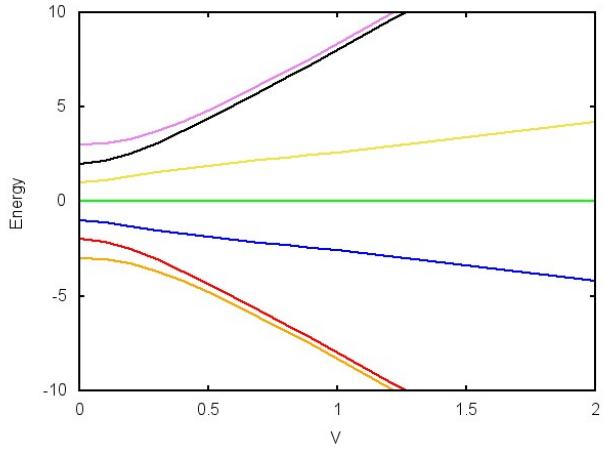

FIG. 2: Energies for the subspace of $k = 3$ versus the interaction term V. This subspace has dimension $2k + 1 = 7$ so we obtain seven different eigenvalues.

easily described using their eigenvectors:

$$\begin{aligned}\hat{K_0}\,|k,m\rangle &= m\,|k,m\rangle\,,\\ \hat{K^2}\,|k,m\rangle &= k(k+1)\,|k,m\rangle\,,\\ \hat{K_\pm}\,|k,m\rangle &= \sqrt{k(k+1)-m(m\pm1)}\,|k,m\pm1\rangle\,.\end{aligned} \tag{5}$$

The quantum number k takes the following values: $0, 1, ..., \frac{N}{2}$ (where N is the number of particles), whereas for each k, m takes the values $-k, -k+1, ..., k$. As we are going to work with an even number of particles, these values will be integers. Every value of k sets up a subspace of $2k+1$ dimension and it will have a definite multiplicity (λ_k). Thus, the total dimension of the space will be the sum of the dimension of each k-subspace multiplied by λ_k. This total dimension is 2^N. We could have also chosen to work with the spin basis. However, it is much more complicated that working with the $|k,m\rangle$ basis. In order to compute the possible k's from the spin values we have to assign to each particle a definite spin ($\frac{1}{2}$ or $-\frac{1}{2}$) and sum all these spins. This will be the m value of this state. The maximum m-value defines the maximum k and can be identified with the state $|k,k\rangle$ with $k = \frac{N}{2}$. Applying successively the operator $\hat{K_-}$ we can express the state in terms of the spin basis. In the same way, the state with all the spins down corresponds to $|k,-k\rangle$ with $k = \frac{N}{2}$. The multiplicity λ_k can be computed with the following equation[10]:

$$\lambda_k = \frac{1+2k}{1+k+\frac{N}{2}}\binom{N}{\frac{N}{2}-k}. \tag{6}$$

k	0	1	2	3	4	5
λ_k	42	90	75	35	9	1
Dim.	1	3	5	7	9	11

TABLE I: Values of the quantum number k, the multiplicity λ_k and the dimension of the subspace for $N = 10$. The sum of the dimension times the multiplicities adds to 2^{10}.

In Table I we provide some values for the dimension and multiplicity of several k-subspaces.

The matrix elements of the Hamiltonian are calculated using Eq. (5):

$$\begin{aligned}\langle k,m|\hat{H}|k,m+2\rangle = -\frac{V}{2}\sqrt{[k(k+1)-m(m-1)]}\\ \sqrt{[k(k+1)-(m-1)(m-2)]},\end{aligned}$$

$$\begin{aligned}\langle k,m|\hat{H}|k,m\rangle &= \epsilon m,\\ \langle k,m+2|\hat{H}|k,m\rangle &= \langle k,m|\hat{H}|k,m+2\rangle\,.\end{aligned} \tag{7}$$

In this work we have focused on a system with an even number of particles. Diagonalizing this Hamiltonian we obtain the energies for the different subspaces. Regarding the energies, one of the keys of the Lipkin model is that the ground state of the system is precisely in the subspace of dimension $N+1$ corresponding to the maximum possible value of k, $k = \frac{N}{2}$. The energies are in units of ϵ to which we have assigned the value of 1. It is obvious that the subspaces with the same k will generate the same values for the energy.

Fig.1 shows the ground state energy as a function of V for different number of particles. We observe that the bigger the number of particles, the more negative the ground state energy is. Also, as the interaction term increases, we notice that these values become more negative. Both facts reflect the attractive character of the interaction term. Notice however, the flatness of the energy when V tends to zero.

Fig. 2 shows the seven energy eigenvalues of the system for $k = 3$ as a function of V. The lowest energy corresponds to the ground state energy for $N = 6$. We can observe that no matter which value takes the interaction term V, the energies of the subspace are symmetric with respect to zero.

III. FINITE TEMPERATURE

A. Formalism

The treatment of the Lipkin model at finite temperature can be done in the canonical ensemble. The partition function Z can be computed after the diagonalization of the Hamiltonian in each of the k-subspaces:

$$Z = \sum_k \lambda_k \sum_{i=1}^{2k+1} e^{-\beta E_i^{(k)}}, \tag{8}$$

where $\beta = \frac{1}{T}$. The Z partition function gives direct access to the free energy:

$$F = E - TS = -Tln(Z), \tag{9}$$

and to the thermal average of the energy:

$$\begin{aligned} E &= \frac{1}{Z}\sum_k \lambda_k \sum_{i=1}^{2k+1} E_i^{(k)} e^{-\beta E_i^{(k)}} \\ &= -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{\partial ln(Z)}{\partial \beta}, \end{aligned} \tag{10}$$

Other quantities of interest are the entropy:

$$S = -\frac{\partial F}{\partial T}, \tag{11}$$

and the heat capacity C:

$$C = \frac{\partial E}{\partial T}. \tag{12}$$

B. Non interacting versus interacting case

In this section we compare the behaviour of the thermodynamic quantities without and with interaction.

We can observe in Fig.3, (a) that for low temperatures the average energy approaches the energy of the ground state. We also notice that the bigger the number of particles, the more negative the ground state energy is.

At high temperatures, the finite size of the Hilbert space, translates in an equiprobable occupation of all energy states of the system. However, this does not explain the zero value of the average energy. In order to give an explanation to this fact we have to focus on the energies of each k-subspace. These eigenvalues are symmetric with respect to zero. Therefore, as at high temperatures all these states are equiprobable, the average energy goes to zero.

Focusing now on the average energy with interaction, Fig.3, (b), we observe the same behaviour at high temperatures as without interaction. The main difference is that in the interacting case the ground state energy is lower. Moreover, with interaction, a higher temperature is necessary to reach the situation of equiprobability, with average energy zero.

We have represented the heat capacity in Fig. 3 (c) and (d) because it is intimately related with the dependence of the energy with temperature. We can observe that at low temperatures, the heat capacity goes to zero in (c) and (d) (independently of the number of particles). Comparing it with the average energy in (a) and (b) we observe that the slope of E versus T is zero and therefore the heat capacity tends to zero. In addition, we can observe that the maximum of the heat capacity in (c) and (d) coincides with the inflection point of the average energy as Eq. (12) requires. In Fig.3, (d), the case with interaction, we observe that depending on the number of particles the maximum is shifted to higher temperatures, meanwhile in the non interacting case in Fig. 2, (c) the maximums are aligned. This shift of the maximum is due to the fact that as the number of particles increases, it is more difficult to reach the inflection point of the energy as a function of T.

The results for the entropy are shown in Fig.3, (e) and Fig.3, (f). On the one hand, without interaction, we can see that as the temperature goes to zero, the entropy tends also to zero as expected (only the lowest energy state is occupied). We can also observe that for a given N, when the temperature increases, the entropy tends to the value $ln(2^N)$, being 2^N the number of microstates. Nevertheless, if we represent the entropy per particle we would have that at high temperatures, no matter the number of particles, the entropy would tend to $ln(2)$. On the other hand, in the interacting case, we observe the same behaviour at high temperatures, but it is more difficult to reach the situation where all the microstates are equally possible. When the temperature is nearly zero, the entropy is also zero as expected. The differences with the case without interaction are observed mainly at low temperatures.

In Fig.3 (g) and (h) we present the results for the free energy. Depending on the number of particles, it takes a more negative value. As temperature rises, Z decreases, so by Eq.(9), the free energy decreases too. As Eq.(9) shows, there is a competition between the entropy and the average energy. As temperature rises, E tends to zero and the term $-TS$ is bigger and more negative, so at high

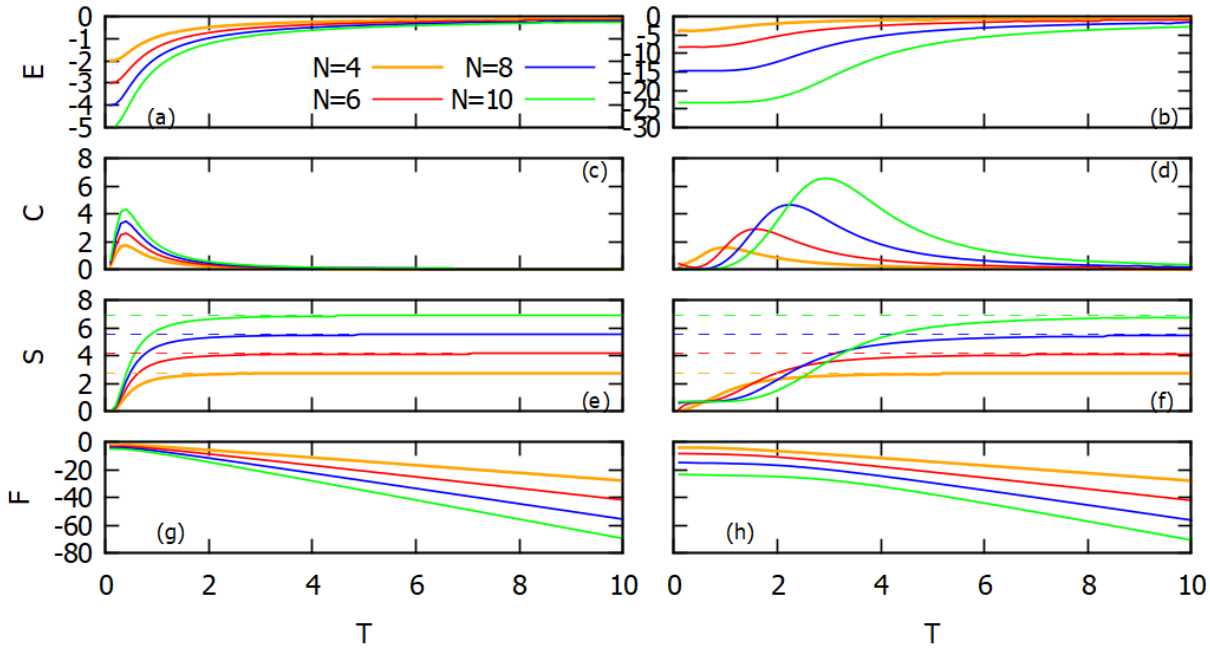

FIG. 3: In the left panel, case without interaction. In the right panel, $V = 1$. (a), (b) E versus T for different N. (c), (d) Heat capacity versus T for different N. (e), (f) Entropy versus T for different N. The dashed line represents the limit at high temperatures. (g), (h) Free energy versus T for different N.

temperatures the free energy is approximately $-TS$. At high temperatures we have proved before that the limit for the entropy is the same with and without interaction so the free energy at high temperatures approaches the same value with or without interaction as observed in (g) and (h). The differences between (g) and (h) are mainly observed at low temperatures. The interaction term V seems to distinguish the values of the free energy depending on the number of particles.

IV. HELLMANN-FEYNMAN THEOREM

The Hellmann-Feynman theorem at $T = 0$ states that if we make a perturbation in our Hamiltonian such that [11]:

$$\hat{H_\lambda} = H_0 + \lambda V, \tag{13}$$

where V is a part of the Hamiltonian. Then the expectation value of V in the ground state can be calculated as:

$$\langle V \rangle_{gs} = \left. \frac{\partial E_{gs,\lambda}}{\partial \lambda} \right|_{\lambda=1}, \tag{14}$$

where $E_{gs,\lambda}$ is the ground state energy of H_λ. This theorem [12] is very useful when the expectation value of V is difficult to calculate but we know how to compute the total energy. In our case, we have numerically checked the fulfillment of the theorem af $T = 0$. In addition, we have extended the Hellmann-Feynman theorem to finite temperature. To this end, we start from the definitions:

$$Z = \mathrm{Tr}[e^{-\beta \hat{H}}], \tag{15}$$

$$F = -T \ln(\mathrm{Tr}[e^{-\beta \hat{H}}]), \tag{16}$$

where Tr is the trace. In one hand, introducing the λ parameter as in Eq.(13) we obtain:

$$F_\lambda = -T \ln(\mathrm{Tr}[e^{-\beta(H_0 + \lambda V)}]). \tag{17}$$

On the other hand we know that the thermal average of V is given by:

$$\langle V \rangle_T = \frac{\mathrm{Tr}(V e^{-\beta \hat{H}})}{\mathrm{Tr}(e^{-\beta \hat{H}})}. \tag{18}$$

Therefore, the derivative of Eq.(17) over λ at $\lambda = 1$ results in:

$$\left. \frac{\partial F_\lambda}{\partial \lambda} \right|_{\lambda=1} = \langle V \rangle_T. \tag{19}$$

Eq.(19) is the extension of the Hellmann-Feynman theorem at finite temperature which states that the

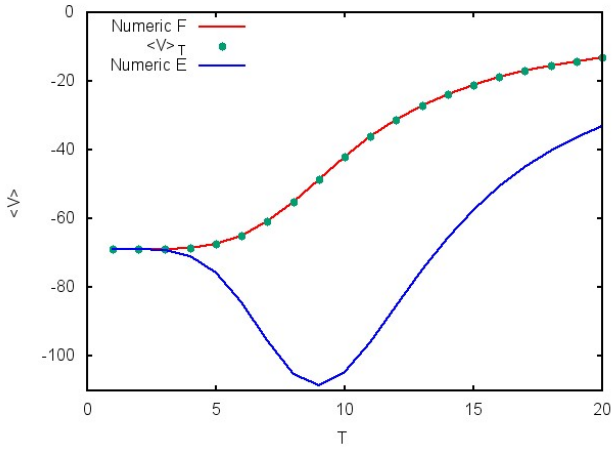

FIG. 4: Results for the Hellmann-Feynman theorem using the derivative of the free energy versus temperature, the average energy versus temperature and also the thermal average of V.

derivative of F with respect to the λ parameter at $\lambda = 1$ coincides with the thermal average of the term V.

As we observe in Fig.4 the direct calculations of the thermal average of $\langle V \rangle$ (circles) coincide with $\langle V \rangle$ calculated according to Eq.(19). Notice the discrepancy when the derivative is calculated with the average thermal energy. This emphasizes the important contribution of the derivative of the entropy with the variation of λ. Obviously, when T tends to zero, as S tends to zero too, the derivative of E_λ and F_λ coincide. The same is true when T becomes large, i.e, when S tends to a constant independent of the interaction.

V. CONCLUSIONS

We have studied the Lipkin model at finite temperature for an even number of particles without and with interaction. We have also studied the Hellmann-Feynman theorem at zero temperature and we have extended it to finite temperature. Our conclusions are:

- The average energy of a system of N fermions tends to the ground state at low temperatures and to zero at high temperatures (all the states are equiprobable) independently of V. This fact is due to the symmetry with respect to zero of the energies of every k-subspace no matter which value takes V.

- The entropy tends to zero at low temperatures and to the logarithm of the number microstates at high temperatures. This behaviour is independent of the interaction term. However, the influence of V is reflected in the temperature at which this value is reached. The bigger the V, the higher the temperature has to be.

- The Hellmann-Feynman theorem at zero temperature states that the derivative of the total energy of the ground state of H_λ at $\lambda = 1$ provides the expectation value of V in the ground state. The extension of this theorem to finite temperature, to obtain the thermal average, $\langle V \rangle_T$, requires to use the corresponding derivative of the free energy, emphasizing the importance of the entropy contribution to $\langle V \rangle_T$.

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[1] H. J. Lipkin, N. Meshkov and A. J. Glick, Nucl. Phys. 62, 188-198 (1965).
[2] S. De Leo and G. Co', Mod. Phys. Lett. A 30 (2015) 1550196.
[3] arXiv:1805.12442v1 [nucl-th] 31 May 2018.
[4] O. Castaños, R. Lopez-Pea, J. Hirsch, E. Lopez-Moreno, Phys. Rev. B74 (2006) 104118.
[5] S. Campbell, G. De Chiara, M. Paternostro, G. Massimo Palma, R. Fazio, Phys. Rev. Lett. 114 (2015) 177206.
[6] N. Debergh, Fl. Stancu, J. Phys. A: Math. Gen. 34(2001) 4267.
[7] S.Y. Tsay Tzeng, P.J Ellis, T.T.S Kuo and E.Osnes, Nucl. Phys. A580(1994)277.
[8] P. Ribeiro, J. Vidal, R. Mosseri, Phys. Rev. Lett. 99(2007) 050402.
[9] K. Hagino, F. Minato, Phys. Rev. C 80 (2009) 047301.
[10] P. Pérez Fernández, PhD: "Estudio de transiciones de fase cuánticas en sistemas de dos niveles", U. Sevilla, 2011.
[11] H. Hellmann, Einfüring in die Quantenchemie (Franz Deuticke, Leipzig, 1937), p. 285.
[12] R. P. Feynman, Phys. Rev. 56, 340 (1936).