Non-equivalence of the microcanonical and canonical ensembles in a bosonic Josephson junction

L.A. González-García
Facultad de Ciencias, Universidad Autónoma del Estado de México (UAEM), Av. Instituto Literario 100, Col. Centro, C.P. 50000, Toluca, Estado de México, México.

R.A. Zamora-Zamora and R. Paredes
Instituto de Física, Universidad Nacional Autónoma de México, Apdo. Postal 20-364, México D.F. 01000, México.

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We investigate the thermodynamic properties of a bosonic Josephson junction in the full quantum approach and, in particular, we concentrate in studying the thermal averages of one- and two-body properties below and above the transition from delocalized to self-trapped regimes. This temperature dependence is determined by using the fact that at equilibrium the microcanonical and canonical ensembles should be equivalent. To establish the robustness of the equilibrium state, we first study a one body property and show numerically that any arbitrary state localized in energy, when evolved, reaches a stationary or equilibrium state. Comparison among averages of one- and two-body properties in the microcanonical and canonical ensembles reveals discrepances, thus leading to non-equivalence among these ensembles. Such averages differences can be attributed to the fact that the Hilbert space of the system scales as its size N, and consequently, the entropy does not scale as N. We further find as a natural consequence of studying the finite bosonic Josephson junction in the two-mode Bose Hubbard context, that positive and negative temperatures are obtained. This result can be generalized for any finite optical lattice.

Keywords: Josephson effect; bosonic Josephson junction; quantum ensemble theory.

Se investigan la propiedades termodinámicas de una junta de Josephson bosónica en la aproximación cuántica de dos modos, en particular, se estudian los promedios térmicos de propiedades de uno y dos cuerpos abajo y arriba de la transición de deslocalización a estado autoatrapado. Esta dependencia en la temperatura se determina usando el hecho que en equilibrio los ensembles canónico y microcanónico deberían ser equivalentes. Primero se establece la robustez del estado de equilibrio estudiando una propiedad de un cuerpo y mostrando numéricamente que cualquier estado arbitrario localizado en energía alcanza un estado estacionario o de equilibrio. La comparación entre promedios de propiedades de uno y dos cuerpos en los esquemas canónico y microcanónico revela descrepancias, exhibiendo así la no equivalencia entre ensembles. Dichas diferencias en los promedios pueden atribuirse al hecho que el espacio de Hilbert del sistema se escala como su tamaño N y consecuentemente la entropía no se escala con N. Adicionalmente, se encuentra como consecuencia natural de estudiar a la junta de Josephson bosónica en la aproximación de dos modos, la existencia de temperaturas negativas. Dicho resultado puede ser generalizado para redes ópticas finitas.

Descriptores: Efecto Josephson; junta de Josephson bosónica; teoría de ensemble cuántico.

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1. Introduction

Today, bosonic Josephson junctions (BJJ) are realizable arrays in ultracold alcaline gases confined in external potentials. The first observation was implemented by Oberthaler ′s group [1] for ^{87}Rb atoms in 2005. Such an array consisted of a sample of $N \sim 10^3$ weakly interacting atoms at $T \sim 10^{-9}$ K, confined in a one dimensional two-well potential. Since then, a variety of Josephson junctions for ultracold atoms, including mixtures of different species of bosons, fermi-boson mixtures, and two- and three-dimensional geometries have been created [2, 3]. The observation of the phase transition from delocalized to self-trapped regimes in these systems is the result of setting a threshold initial population in each well for a constant interparticle interaction, or manipulating both, the geometry of the two-well potential (varying the potential depth), and the interparticle interaccions (by changing the $s-$wave scattering length externally).

In parallel to the experimental understanding of BJJ, the theoretical approaches addressing those systems, have provided a reasonable description of both the dynamical behavior and the phase transition from the delocalized (or coherent transport) to the self-trapped regime, as a function of the parameter that characterizes the interparticle interaction and of the initial many-body state. Those two-mode descriptions [4–15, 17, 18] are the mean field approach based on the Gross-Pitaevskii equation and the full quantum description circumscribed in the second quantized frame. Although these theories predict the occurrence of the transition from delocalized to self-trapped transition as a function of the two-particle interaction and the initial condition, it is important to remark that the exact quantum description *vs* the mean field approach supplies a more general description of the system since in principle $N-$body properties can be investigated from such an scheme. As a matter of fact, the property of dynamical stationarity detected from few body quantities [15,19,20] can only be established from full quantum calculations from the entire landscape of energy and interparticle interaction energy.

Since a BJJ array is a closed system with a fixed number of particles N where a given inital state fixes the total energy ϵ for a constant interaction strength, a microcanonical ensemble is the natural one to describe the average or expectation value of few body properties. Thus, the eigenstates of the Hamiltonian modelling a BJJ array would be the proper states to describe the average or expectation value of any arbitrary few body property. There exists however, as indicated by previous studies [19, 20], states that give rise to dynamical stationary, or equilibrium, values in few-body properties, whose average coincides with the expectation value of those few-body properties in the eigenstates. Those are the well known family of coherent states [21, 22] that have the property of possessing small energy mean-square deviation, that is, they are states localized in energy. Thus, for a given number of particles and by considering such coherent states, a microcanonical ensemble defined by the variables N and ϵ can be set. The equilibrium values in this ensemble will be used to determine its associated thermal averages in the canonical ensemble.

Although it is not necessary to over emphasize the importance on the temperature dependence of the thermodynamic properties in a macroscopic system, it is important to point out that a very important issue in the ultracold systems is the thermometry. Typically, temperatures are obtained from theoretical adjustable models to in situ density profiles, or by other indirect methods [23]. For the particular case of BJJ, the temperature can be presumably extracted from the used model describing this system, namely the two-mode Bose-Hubbard model. However, as we shall see, the non-equivalence between canonical and microcanonical schemes in this systems, leaves still open the question of the temperature determination. Perhaps the model describing BJJ must be reconsidered and make the necessary adjustments to circumvent the failure pointed here. As we shall argue in section III, one of the rutes to extend the two-mode Bose-Hubbard model is to include not just the lowest two modes, but the next two energy levels and its corresponding localized wave functions.

The purpose of this work is to investigate the thermal averages of one- and two-body properties in a BJJ array, below and above the transition from delocalized to self-trapping regimes in the canonical ensemble. Such functionality will be established by using the fact that at equilibrium the microcanonical and canonical ensembles should be equivalent, and therefore, it should be possible to describe the average value of few-body properties in both the microcanonical ensemble defined by the variables (ϵ, N) and in the canonical ensemble defined by the variables (T, N). In particular, we shall concentrate in studying the temperature dependence of the particle population in each well $\langle \hat{N}_i \rangle$ and of the tunneling correlation $\langle \hat{\mathcal{C}} \rangle = \langle (b_1^\dagger b_2 + b_2^\dagger b_1)^2 \rangle$. We shall find that the predictions of the different ensembles do not agree with each other.

This article is organized as folllows. In section II we introduce the model Hamiltonian and show that a BJJ exhibits the property of dynamical stationarity for any arbitrary value of the parameter characterizing the interaction among the particles and for any initial many-body state, through the study of a one-body property when arbitrary coherent states are evolved in time. In section III we study the particle population and the tunneling correlation (one- and two-body properties respectively) in the canonical ensemble, and show that even in the thermodynamic limit, the BJJ system exhibits the non-equivalence between microcanonical and canonical ensembles since the few-body averages differ. As we shall discuss, such discrepancies may be attributed to the fact that the size of the Hilbert space of the system scales as N instead of e^N. This same feature of reduced Hilbert space, allow us also to show that negative and positive temperatures consistent with the thermodynamic second law are obtained. Finally in section IV a summary with the main results is presented.

2. The Hamiltonian in the microcanonical ensemble

To model BJJ we work in the full quantum frame considering the two-mode approximation, that is, the two-mode Bose-Hubbard model. Derivation of this Hamiltonian can be found elsewhere [6, 7, 10, 15]

$$\hat{\mathcal{H}} = -\frac{\Delta}{2}\left(b_1^\dagger b_2 + b_2^\dagger b_1\right) + U\left(b_1^\dagger b_1^\dagger b_1 b_1 + b_2^\dagger b_2^\dagger b_2 b_2\right). \quad (1)$$

The parameter Δ is the energy spacing of the two lowest energy modes in a symmetrical two well potential and $U = 4\pi\hbar^2 a/m$ represents the effective particle-particle interaction strength written in terms of the (positive) s-wave scattering length a. As previously pointed in the literature [15, 16], Hamiltonian (1) assumes that the overlap among localized single-wave functions is neglected and therefore the effective interaction among particles occurs only whenever the particles move within the same well. We use units with $\hbar = \Delta = m = 1$.

The microcanonical ensemble is defined by specifying the number of particles N and the expectation value of the energy ϵ. As mentioned in section I, alternatively to the eigenstates of Hamiltonian (1), the coherent states [21, 22] are suitable states to set the variables defining the microcanical ensemble since they possess small energy mean square deviation. Those states written in the atom number basis or Fock states $|N_1, N_2\rangle$, where N_1 and N_2 ($N_1 + N_2 = N$) is the number of particles in wells 1 and 2, are defined as follows:

$$|\theta, \phi\rangle = \sum_{N_1=0}^{N} \binom{N}{N_1}^{1/2} \sin^{N-N_1}(\theta/2) \times \cos^{N_1}(\theta/2)\, e^{-i(N-N_1)\phi} |N_1, N - N_1\rangle. \quad (2)$$

The angles θ and ϕ define a particular initial state, that is, a particular energy ϵ. These angles can be determined by fixing the expectation value of the energy or the initial population in, say, well 1. In fact, in a previous work [20] it has been shown that such states behave as the eigenvectors of Hamiltonian (1) when θ and ϕ are properly chosen, in the sense that the expectation value of a few-body property in the eigenstates, coincides with the averaged equilibrium or stationary state of the same property in the coherent states.

By considering any of the coherent states (2) as the initial one for the system, one can evolve it numerically [24], $|\theta, \phi; t\rangle = \exp(-i\hat{\mathcal{H}}t/\hbar)|\theta, \phi\rangle$, and calculate the expectation values of the observables $\hat{N}_1$, the particle population in well one, and $\hat{C} = \left(b_1^\dagger b_2 + b_2^\dagger b_1\right)^2$, the tunneling correlation,

$$\langle \hat{N}_1(t)\rangle_\tau = \langle \theta, \phi; t|\, \hat{N}_1\, |\theta, \phi; t\rangle \tag{3}$$

and

$$\langle \hat{\mathcal{C}}(t)\rangle_\tau = \langle \theta, \phi; t|\, \hat{\mathcal{C}}\, |\theta, \phi; t\rangle, \tag{4}$$

where the time interval τ in which the average is taken corresponds to the interval of time where the stationarity is observed [20]. Even in a closed system, the property of stationarity is very difficult of being captured from the information enclosed in a $N-$body system, however, it can be observed directly from the expectation value of few body properties [15, 19]. To show that any state belonging to the family of coherent states reaches an equilibrium state when few-body properties are studied, we followed the evolution in time of the expectation value of the particle population $\hat{N}_1$ in the coherent states (2) taking $0 < \theta < 2\pi$ and $0 < \phi < 2\pi$. In Fig. 1 we show the stationary values of the particle population in well 1, N_1 , in the family of coherent states $|\theta, \phi; t\rangle$, as a function of their expectation value of the energy $\epsilon(\theta, \phi)$, for N = 1000 [24].

For purposes of calculations of the stationary states, we selected a specific value of the parameter $\Lambda = UN/\Delta$ ($U = 1.1, \Delta = 1$ and $N = 1000$) and follow the evolution of the chosen states for times longer than the time spent in the stationary state, $t \gg \tau$. As has been pointed out in

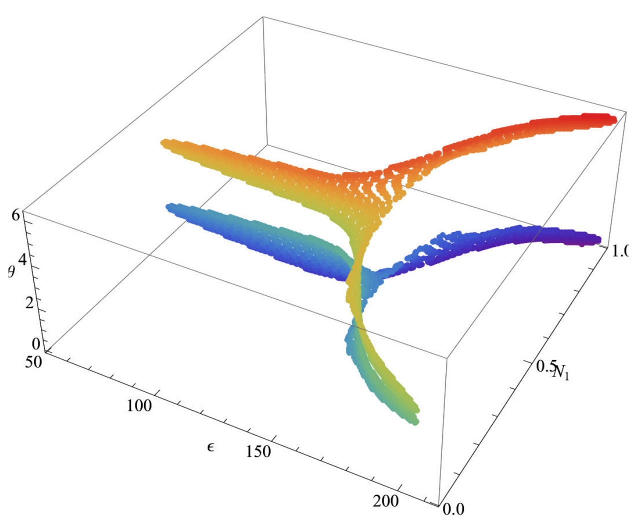

FIGURE 1. Statistically stationary values of the number of particles in well 1, N_1^s , in the family of coherent states $|\theta, \phi; t\rangle$, as a function of their expectation value of the energy $\epsilon(\theta, \phi)$, for $N = 1000$.

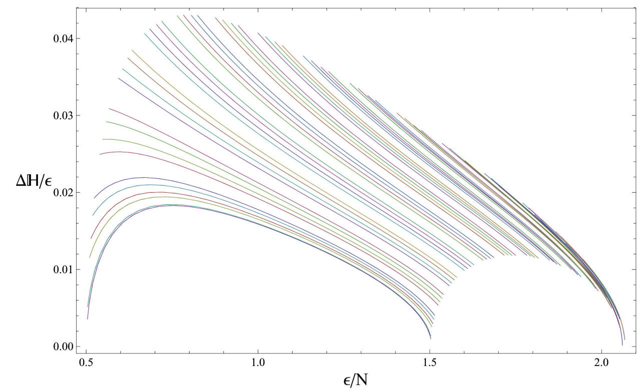

FIGURE 2. Energy mean square deviation for $N = 1000$, $\Lambda = 1.1$, for the values of θ and ϕ in Fig. 1.

the literature [7–9, 11–15, 18], for any value of the interaction parameter Λ, and for any initial condition, the particle population shows the phenomenon of collapses and revivals in the many-body dynamics. However, it is important to remark that if we observe the system for a long but arbitrary time, it will mostly be found in the stationary state. Thus, the rubustness of the stationarity is verified. To complement the information encoded in Fig. 1, we plot in Fig. 2 the energy mean-square deviation $\Delta\mathbb{H} = \sqrt{\langle \mathcal{H}^2\rangle - \langle \mathcal{H}\rangle^2}$ for $N = 1000$, $\Lambda = 1.1$, for the values of θ and ϕ in Fig. 1. As expected, the set of coherent states appear to be localized in energy.

3. Thermodynamical properties in the canonical ensemble

To discuss the role of the temperature in BJJ, and particularly, to determine the dependence of the average values of few body properties on the temperature, we should first recall that such an isolated system is, as stated in section I, described by a microcanonical ensemble. Namely, its macroscopic state is characterized by the number of particles N and the energy ϵ. Depending on the values of these variables, and if the system is in equilibrium, it should have a well defined temperature $T = T(N, \epsilon)$. If in the thermodynamic limit the ensembles are equivalent, one should obtain the same results for the equilibrium states using the canonical ensemble with N and T given. Due to the simplicity of the system under study, one can very easily calculate the average value of any observable operator $\hat{A}$ in the canonical ensemble,

$$\langle \hat{A}\rangle = \frac{1}{Z}\sum_{n=0}^{N} \langle \phi_n|\hat{A}|\phi_n\rangle\, e^{-\varepsilon_n/kT}, \tag{5}$$

where k is Boltzmann constant and the partition function is

$$Z = \sum_{n=0}^{N} e^{-\varepsilon_n/kT}. \tag{6}$$

With this procedure, and assuming that the temperature is a single valued function of N and ϵ, we can assign a temperature to a stationary state with a given energy ϵ by solving the following equation for T,

$$\epsilon = \frac{1}{Z}\sum_{n=0}^{N} \varepsilon_n \, e^{-\varepsilon_n/kT}. \qquad (7)$$

To determine the thermal averages of $\hat{N}_1$ and $\hat{\mathcal{C}}$ by means of Eq.(5) as a function of T and N, we proceed as follows. We solve the eigenvalue system (1) for values of Λ below and above the transition $\Lambda = 0.1$, 1.0 and 10.0, that is, we find the eigenenergies ε_n

$$\hat{\mathcal{H}}(\Lambda)|\phi_n(\Lambda)\rangle = \varepsilon_n(\Lambda)|\phi_n(\Lambda)\rangle.$$

From the analysis done in section I, we selected the values of θ and ϕ such that for a given value of Λ the condition

$$\epsilon(\theta, \phi) = \varepsilon_n,$$

is satisfied, that is, we determine the values of θ and ϕ defining the coherent state for the entire energy spectrum ε_n for $\Lambda = 0.1$, 1.0 and 10.0. Then, by solving eq. (7) we determine the temperature T in the canonical ensemble associated to the microcanonical ensemble defined by ϵ and N. All the calculations presented in this work were done for $N = 1000$. It is worth to mention that we verified that calculations for $N = 10^4$ give esentially the same results. Thus, the assumed equivalence among microcanoical and canonical ensembles is well justified.

By means of equation (5) we determine the thermal averages of $\hat{N}_1$ and $\hat{\mathcal{C}}$. The gray dotted and black dashed curves in Fig. 3 correspond to the averages of $\hat{N}_1$ in the eigenstates and in the coherent states respectively, while the black solid line is the average of N_1 in the canonical ensemble. Analogously, the gray dotted and black dashed curves in Fig. 4 correspond to the averages of $\hat{\mathcal{C}}$ in the eigenstates and in the coherent states respectively, while the black solid line is the average of $\hat{\mathcal{C}}$ canonical ensemble.

Regarding the results obtained for $\langle \hat{N}_1 \rangle$ we observe that there is no agreement between the microcanonical and the canonical descriptions above the transition from delocalized to self-trapped regimes, that is, we find that the thermal average of $\hat{N}_1$ is essentially equal to $N/2$, whether above or below the transition, while taking the average in the microcanonical ensemble allows us to detect the transition. Such a discrepancy can be interpreted as the impossibility of showing spontaneous symmetry breaking. This phenomenon is analogous to the fact that in the Ising model in 2D the average magnetization is always zero: one needs a small external magnetic field to break the symmetry and then make it to vanish [25].

The behavior of the average values of the two-body tunneling correlation $\hat{\mathcal{C}}$ reveals also discrepancies between canonical and microcanonical ensembles. As in the particle population case, the transition from delocalized to self-trapped states (the peaks in gray dotted lines in Fig. 4) is not observed in the thermal averages (black solid lines). We do not have an explanation for such a discrepancy. It may either be that our calculation based on the coherent states do not correspond to a microcanonical ensemble, or that for this system there is simply no equivalence between ensembles. This possibility can be explained as follows. The system under study is peculiar in the sense that it represents a collection of atoms interacting with the same strenght with all the other atoms, provided they are in the same internal state. In other words, the fact of considering the two-mode approximation only, has given rise to an effective Hamiltonian in which the interactions among the particles appear as if they were long range, whenever the particles have the same internal state, while the full Hamiltonian represents particles with short range interactions. Moreover, it can also be shown, by studying Eq.(7), that the energy as a function of temperature and number of particles is not fully extensive, namely, it is not of the form $\epsilon(T, N) = N\, e(T)$ with $e(T)$ a function of the energy only, but rather, $\epsilon(T, N) = Ne(T/N)$. The two-mode approximation reduces dramatically the Hilbert space of the N-body system and consequently the extensive character of the thermodynamic variables with such intrinsic nature is lost.

As it is well known, the entropy of a macroscopic system in equilibrium scales as e^N, and thus its extensivity is reflected along several thermodynamic properties. Nevertheless, a system having a small equilibrium landscape, gives rise to non-extensive thermodynamics. As stated above, the two-mode Bose-Hubbard Hamiltonian causes such behavior. It is important to emphasize however that the n-mode models used to describe 1D finite optical lattices could not have reduced Hilbert spaces, giving rise therefore to recover the extensive character of the natural extensive properties.

In the study of BJJ an alternative to circumvent the found discrepancies among canonical and microcanonical schemes, is the inclusion the next energy band. That is, instead of considering the first energy band with the two lowest energy levels, perform the analysis taking into account the second energy band, and thus dealing with a Hamiltonian in the four-mode approach. The eigenstates analysis of a Hamiltonian with an such an extension has already been addressed in [28] , where, as stated, the Hilbert space scales as $(N + 1)(N + 2)/2$. Thus, by extending the available Hilbert space one could find that such differences are diminished.

In addition to the analysis presented above we should stress an important point regarding the dependence of the temperature T on the energy ϵ in a BJJ. Since those systems are modelled by means of a two-mode approach and consist of a finite number of particles, they exhibit negative temperatures [26]. This fact is compatible with the thermodynamic second law in the sense that heat flows from a negative temperature T_1 to a positive temperature T_2, whenever the energies associated to T_1 and T_2 fulfill the condition $\epsilon_1 < \epsilon_2$. To illustrate this behavior, in Fig. 5 we plot the inverse of the temperature as a function of ϵ for $N = 1000$ and $\Lambda = 0.1$. It is important to note that this figure is consistent with the third law of thermodynamics since $1/T$ is never reached. In general one can state that every finite system with a bounded

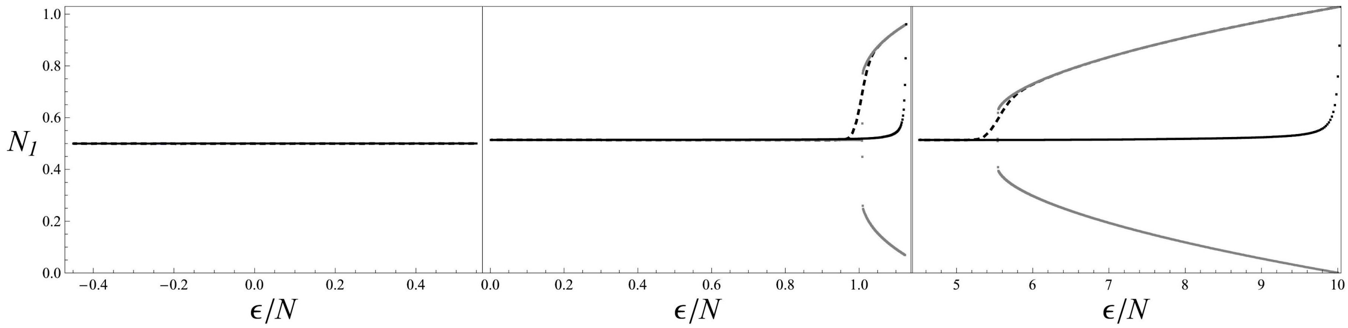

FIGURE 3. Averages of $\hat{N}_1$ as a function of Λ, Λ =0.1(left), 1.0(center) 10.0(right). The gray dotted and black dashed lines correspond to the averages of $\hat{N}_1$ in the eigenstates and in the coherent states respectively, while the black solid line is the average of $\hat{N}_1$ in the canonical ensemble Calculations were performed using $N = 10^3$.

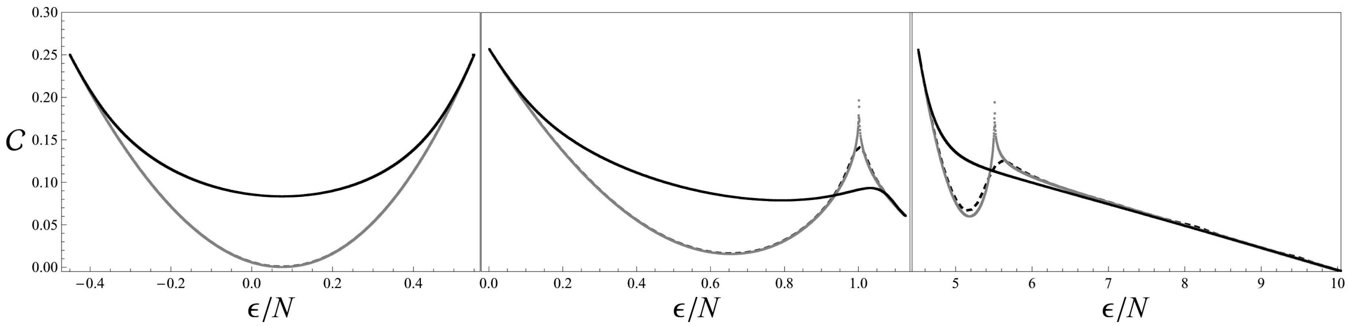

FIGURE 4. Averages of $\hat{\mathcal{C}}$ as a function of Λ, Λ =0.1(left), 1.0(center) 10.0(right). The gray dotted and black dashed lines correspond to the averages of $\hat{\mathcal{C}}$ in the eigenstates and in the coherent states respectively, while the black solid line is the average of $\hat{\mathcal{C}}$ in the canonical ensemble. Calculations were performed using $N = 10^3$.

energy spectrum exhibits negative temperatures. Thus, in the light of the experiments performed in optical lattices, the knowledge of this fact, provides a tool to use such a systems as a reservoir with externally controlable temperature.

4. Conclusions.

We have addressed the thermodynamic properties of an interacting $N-$body boson fluid confined in a double well potential in one dimension. In particular, we concentrate in studying the thermal averages of one- and two-body properties. This study was motivated by the experimental realization of a single bosonic Josephson junction (BJJ) in two weakly linked Bose-Einstein condensates. Such an array can be considered as a closed system with a well defined energy fixed by means of adjustable external parameters. Thus, the natural ensemble to describe a BBJ array is a microcanonical ensemble-like. To model the BJJ array in the microcanical ensemble, we use the two-mode Bose-Hubbard Hamiltonian, and show that for every definite value of the energy, the equilibrium state in the system can be established by following the dynamical evolution in few-body properties until stationarity is reached. The family of coherent states, which are states localized in energy, allowed us to show numerically that any arbitrary initial state, that is, any fixed energy value defining a microcanonical ensemble-like, reaches a statistically stationary state. Our calculations were done for 10^3 particles whose interaction was characterized by a parameter $\Lambda = NU/\Delta$ responsible, together with the initial state, for the transition from delocalized to self-trapping regime. By assuming that at equilibrium the microcanonical ensemble, defined by the variables (N, ε), and canonical ensembles are equivalent, we determine the temperature T associated to each equilibrium state. We further determine the thermal av-

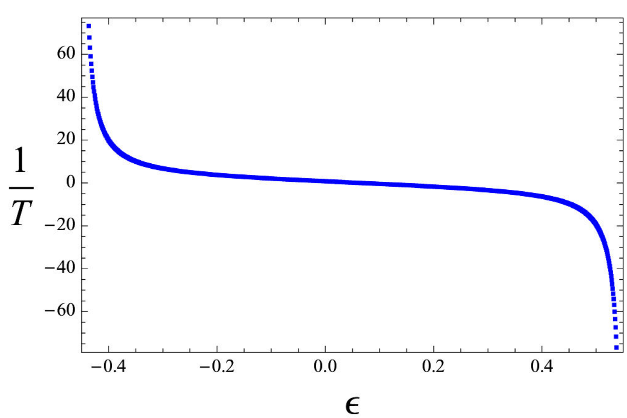

FIGURE 5. Inverse of temperature as a function of ϵ. Calculations were performed using $\Lambda = 0.1$ and $N = 10^3$.

erages of the particle population in each well $\langle \hat{N}_i \rangle(T)$ and the tunneling correlation $\langle \hat{\mathcal{C}} \rangle(T) = \langle (b_1^\dagger b_2 + b_2^\dagger b_1)^2 \rangle(T)$. From the analysis for the particle population study we found that there is no agreement between the microcanonical and the canonical descriptions above the transition from delocalized to self-trapped regimes, in other words, we observed that the thermal average of $\hat{N}_1$ is essentially equal to $N/2$, whether above or below the transition, while taking the average in the microcanonical ensemble allows us to detect the transition that below the transition. Regarding the thermal averages of the tunneling correlation $\langle \hat{\mathcal{C}}(T) \rangle$, we observed that either, below and above the transition, the microcanonical and canonical descriptions are non equivalent. One can attribute this result to the fact that in a BJJ array the entropy does not scales as e^N but as N, as a consequence of being a finite two-level system.

Acknowledgments

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