Entanglement of alkaline-earth-metal fermionic atoms confined in optical lattices

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We calculate the entanglement of the ground state of alkaline-earth-metal fermionic atoms confined in one-dimensional optical lattices. This system can be described using the Kondo lattice model plus a harmonic confining potential, and we adopt the density-matrix renormalization group to study its ground state. We find that the local von Neumann entropy is constant in the insulating domains, and a one-to-one correspondence with the variance of the local density is observed. We show that the average entropy and its derivative are useful tools for identifying quantum transitions in impurity systems.

I. INTRODUCTION

During the last decade, it was shown that some measures of entanglement are useful tools for identifying quantum critical points in strongly correlated systems [1]; today, this has become an alternative route because the critical point can be localized without *a priori* knowledge of the nature of the transition. However, the relationship between entanglement and quantum criticality is not completely clear, since some measures provide information about the critical point and others do not on the same system.

The experimental measure of entanglement is a very important goal in physics today. Some proposals have considered protocols based on appropriate quantum quenches in one-dimensional systems [2]. Macroscopic magnetic measurements have also been performed in order to detect and characterize field-induced quantum entanglement in low-dimensional spin systems [3].

The entanglement in impurity systems that experience the competition between the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions has also been analyzed in recent years. In elliptical quantum corrals with impurities in the foci, the von Neumann entropy between the conduction electrons in the ellipse and the impurities allows one to identify the Kondo and the RKKY regimes [4]. Cho and McKenzie [5] calculated the concurrence, negativity, and von Neumann entropy for the two-impurity Kondo model and found that a minimum nonzero correlation between both impurities is needed for them to create an entangled state. For a spin-chain Kondo model in the Kondo regime, Bayat *et al.* [6] determined the spatial extent of the Kondo screening cloud using negativity. Mendoza-Arenas *et al.* [7] observed that the block entropy of the Kondo necklace model presents a maximum at the quantum critical point between an antiferromagnetic and a Kondo singlet state.

In this paper, we study the ground state of the Kondo lattice model with a harmonic potential using the von Neumann entropy measure of entanglement. This model describes alkaline-earth-metal fermionic atoms confined in one-dimensional optical lattices [8].

II. MODEL

Recently, Fukuhara *et al.* [9] achieved a degenerate Fermi gas with ^{173}Yb atoms, and Daley *et al.* [10] showed that the $^1S_0$ (g) and $^3P_0$ (e) states of alkaline-earth metal can be confined independently in two different optical lattice potentials with the same periodicity. At low temperatures, the scattering lengths for the states $|ee\rangle$, $|gg\rangle$, and $\frac{1}{\sqrt{2}}(|eg\rangle \pm |ge\rangle)$ are independent of the nuclear spins, which guarantees that there will not be any spin-changing collisions. When the strong repulsion between e atoms is taken into account through a unit-filling constraint, and considering that they are localized, it is possible to describe the system by the Hamiltonian

$$H = -t \sum_{i\sigma}(c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) + J \sum_i \mathbf{S}_{ic} \cdot \mathbf{S}_{if}$$
$$+ V \sum_i \sum_{\sigma=\uparrow,\downarrow} \left(i - \frac{L+1}{2}\right)^2 n_{i\sigma}, \qquad (1)$$

where, in standard notation, i varies along the sites of a one-dimensional lattice of size L, $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an atom at site i in the electronic state $^1S_0$, and (nuclear) spin state $\sigma = \uparrow$ or $\downarrow$, and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. In the Hamiltonian (1), $\mathbf{S}_{if}$ is a localized spin-$\frac{1}{2}$ operator, and $\mathbf{S}_{ic} = \frac{1}{2} \sum_{\alpha\beta} c_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{i,\beta}$ is the delocalized atom spin-density operator, where $\boldsymbol{\sigma}$ is the vector of 2×2 Pauli matrices. The quadratic potential term in the Hamiltonian was included in order to consider the delocalized atoms' confining potential due to the trap, and the strength parameter V chosen must, in numerical simulations, be large enough to assure that there are no atoms at the edges of the chain. In the Hamiltonian (1), the hopping integral t is set to 1, and we assume that the lattice constant is equal to 1.

Foss-Feig *et al.* [11,12] studied the above model using mean-field theory with a local-density approximation and found that metallic and Kondo insulator domains coexist. A beyond-mean-field treatment was made by Silva-Valencia and Souza [13], who determined the state diagram of the model.

We used the density-matrix renormalization group method [14] with open boundary conditions to study the Hamiltonian (1). We kept up to $m = 600$ states per block and obtained a discarded weight around 10^{-7} or less.

III. RESULTS

The effect of a harmonic potential in one-dimensional bosonic or fermionic systems is to generate an inhomogeneous distribution of particles in the lattice. This fact leads us to
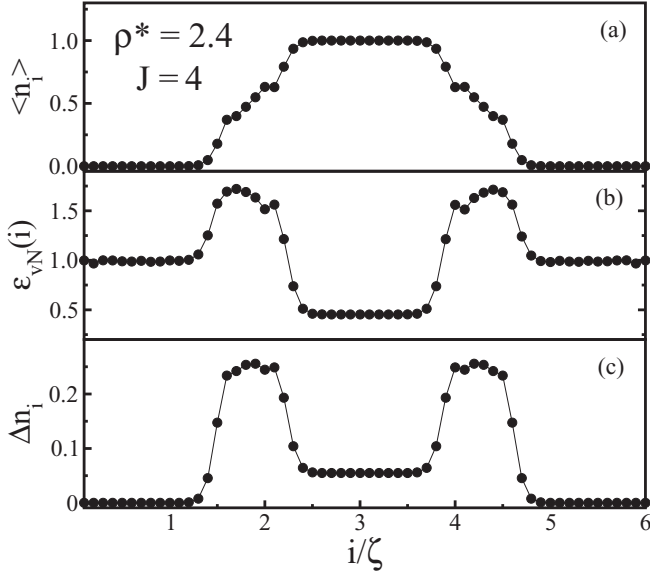
FIG. 1. (a) Local-density profile, (b) local von Neumann entropy, and (c) variance of the particle density of alkaline-earth-metal fermionic atoms confined in an optical lattice. The parameters involved are $L = 60$, $N = 24$, $J = 4$, and $V/t = 0.010$.

consider expected values of local quantities in order to study the ground state of these systems. The first local quantity considered is the local density $\langle n_i \rangle = \langle \sum_\sigma n_{i\sigma} \rangle$.

Due to the slow convergence of the inhomogeneous Hamiltonian (1), in this paper we consider lattice sizes up to $L = 60$. In Fig. 1(a), we show the density profile of $N = 24$ delocalized atoms trapped in an optical lattice of strength $V/t = 0.010$. Here the antiferromagnetic coupling is $J = 4$. So that our results are independent of the particular filling and lattice size, we use the characteristic length $\zeta = (V/t)^{-0.5}$ and the characteristic density $\rho^* = N(V/t)^{0.5}$ in the description of our results. In Fig. 1(a), we have $\rho^* = 2.4$, and observe that the local density is zero around the ends of the system; therefore, all atoms are confined in the trap. Then the local density increases and reaches the value $\langle n_i \rangle = 1$, remaining constant around the middle of the trap. The external flat regions in the density profile are insulating regions, since there are not any charge fluctuations, and the middle flat region could be a "Kondo insulator" region, remembering that the homogeneous system at the half-filling case ($\langle n_i \rangle = 1$) presents a charge and spin gap, which is a phase commonly called the Kondo spin-liquid phase. However, the description of the middle flat region requires the calculation of the other local quantities. Now, we consider the local von Neumann entropy defined by

$$\varepsilon_{vN}(i) = -\mathrm{Tr}\rho_i \log_2 \rho_i, \quad (2)$$

where $\rho_i = \mathrm{Tr}_B \rho$ is the density matrix of a single site located at i, whereas B represents the environment with $L - 1$ sites, and ρ is the density matrix of the whole system.

The profile of the local von Neumann entropy is shown in Fig. 1(b). This quantity is constant in the "band insulator" regions without atoms, and its value is 1. In these regions, we have only two possible states at each site: nondelocalized atoms with localized ones with spin up or spin down. In metallic regions with particle density $\langle n_i \rangle < 1$, the degree of

freedom at each site increases, and the entanglement follows this tendency, $\varepsilon_{vN}(i) > 1$. In the middle of the trap, the density particle is constant and equal to $\langle n_i \rangle = 1$, and the local delocalized and localized atoms form singlets, decreasing the degree of freedom, which is a fact that is clear from the figure, whereas the local von Neumann entropy reaches its minimum value in this region.

In order to characterize insulating regions of particles confined in a trap, it is common to use the variance of the local density ($\Delta n_i = \langle n_i^2 \rangle - \langle n_i \rangle^2$) [15,16], which is shown in Fig. 1(c). We see that the variance is zero in the band-insulator regions, reflecting the absence of fluctuations; in the metallic regions, the variance of the local density is different from zero, whereas in the middle of the trap the variance is constant. The constant value of the variance of the local density in the Kondo insulator domain indicates the presence of an incompressible, insulating region where the local compressibility $\kappa_i = \partial n_i / \partial \mu_i = \beta \Delta n_i$ drops to a small but finite value. It is important to emphasize that while the confined system has locally incompressible regions, the global compressibility is never zero, and no true phase transition can occur.

In Fig. 1, we observe that flat regions of the variance of the local density are in one-to-one correspondence with flat regions of the local von Neumann entropy profile; i.e., insulating regions can be described by domains with a constant value of the local von Neumann entropy. Similar results were found by França *et al.* [17] and Silva-Valencia *et al.* [18] for fermions confined in an optical lattice.

We show, in Fig. 2, the evolution of $N = 48$ alkaline-earth-metal fermionic atoms as a function of the confining potential with a fixed local coupling $J = 4$. In Figs. 2(a) and 2(d), the local density and the von Neumann entropy are shown for $V/t = 0.010$ ($\rho^* = 4.80$). We observe that the increase in the delocalized atoms increases the Kondo insulator domain and the effective confined region. As the confining potential increases, $V/t = 0.019$ ($\rho^* = 6.62$), a metallic region appears in the middle of the trap, and the Kondo insulator domains
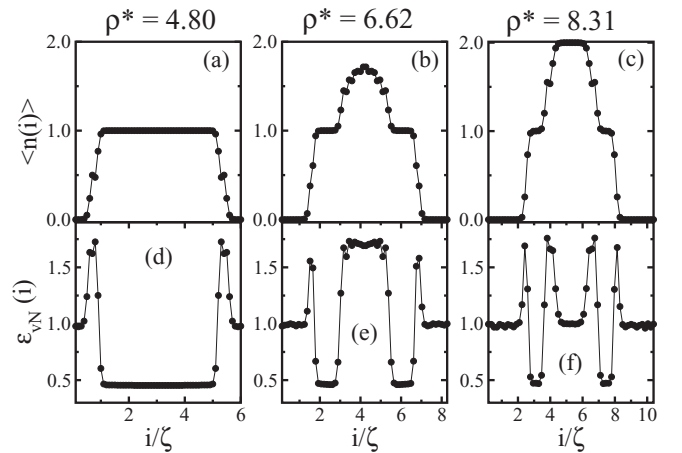

FIG. 2. (a)–(c) Local density profile, and (d)–(f) local von Neumann entropy, for $N = 48$ delocalized fermions interacting with a local coupling $J = 4$ for different characteristic densities. The confining potential is $V/t = 0.010$, $V/t = 0.019$, and $V/t = 0.030$ for plots in the first, second, and third column, respectively.

decrease [see Fig. 2(b)]. In the central metallic region, the degree of freedom increases and the local von Neumann entropy takes larger values, as can be seen in Fig. 2(e). A band-insulator region appears as $V/t = 0.030$ ($\rho^* = 8.31$), which coexists with metallic regions and Kondo insulator domains, as can be seen in Fig. 2(c). In this band insulator, each site has only two states: a fully occupied site with a localized atom with spin up or spin down; therefore, the local von Neumann entropy value is 1. We also note that the local von Neumann entropy value at the Kondo insulator domain is almost independent of the confining potential, and the confined region decreases with the confining potential.

From Figs. 1 and 2, we observe that the local von Neumann entropy is equal to 1 in the band-insulator regions, and takes a lower value at the Kondo insulator domain. These facts, and the above discussion, allow us to conclude that the local von Neumann entropy is a useful quantity for describing the ground state of alkaline-earth-metal fermionic atoms confined in optical lattices.

To study fermions in spatially inhomogeneous systems, França and Capelle [17] proposed a local-density approximation to the von Neumann entropy, in which the entanglement functional is approximated by evaluating the per-site entropy of the homogeneous system at the density distribution of the inhomogeneous system. They showed that the entanglement and its derivative are useful tools for describing the state transition of fermions confined in one-dimensional optical lattices. Following their proposal, we also calculate the average per-site entropy, $\varepsilon^* = \frac{1}{L} \sum_i \varepsilon_{vN}(i)$.

Figure 3 displays the average per-site entropy ε^* and its derivative as a function of the curvature of the trapping potential. When the confining potential increases, the Kondo insulator domain decreases, while the external band-insulator growth and the average entropy decrease. This scenario

changes when a metallic region appears in the middle of the trap, increasing the local degree of freedom in this region; i.e., the entanglement increases, as can be seen in Fig. 3(a). We observe that the change in the ground state generates a jump in the average entropy. A subsequent increase in the confining potential decreases the size of the Kondo insulator domains, increasing the metallic regions, which is reflected in an increase in the average entropy. However, the increase in the filling around the middle of the trap is accompanied by a gradual decrease in the local entropy there. Therefore, we do not observe a strong change in the average entropy; as the band insulator appeared with fully occupied sites, only a small decrease was seen around $V/t \approx 0.027$. For bigger values of the confining potential, we expected that the average entropy tends to 1 because the Kondo insulator domain would disappear.

The distinctive features of the average entropy curve, showing changes in the ground state, are seen more clearly in the derivative of the average entropy, which is shown in Fig. 3(b). A spike in the derivative signals the appearance of a metallic region in the middle of the trap, and the transition point is at $V/t = 0.013$. After a few regular evolutions, we observe a smaller peak at $V/t = 0.027$, which is associated with the formation of a band-insulator region with fully occupied sites in the middle of the trap.

Figure 3 shows us that the average entropy and their derivative are useful tools for identifying the transition points where the ground state of alkaline-earth-metal fermionic atoms confined in optical lattices changes.

The local von Neumann entropy profile of a system with $N = 48$ delocalized atoms, characteristic density $\rho^* = 8.31$, and two different antiferromagnetic couplings ($J = 6$ and 9) is shown in Fig. 4(a). We observe that the local coupling kills the band-insulator region at the center of the trap and favors
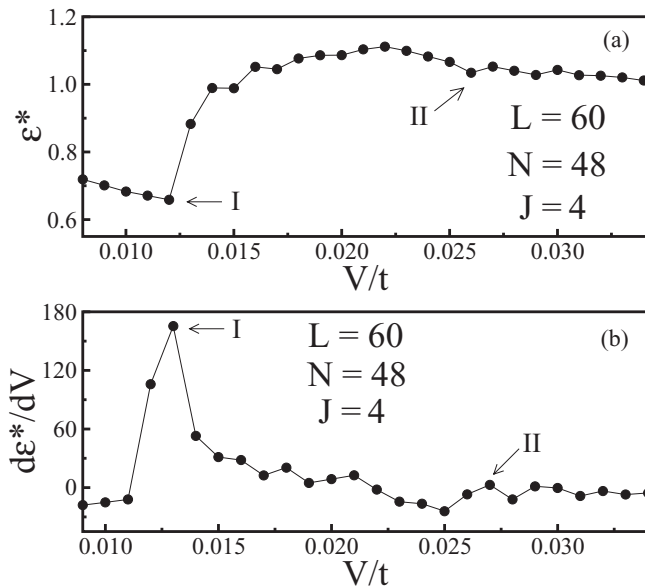

FIG. 3. (a) The average von Neumann entropy and (b) its derivative as a function of the confining potential. The parameters involved are $L = 60$, $N = 48$, and $J = 4$. I and II mark where the transitions take place.
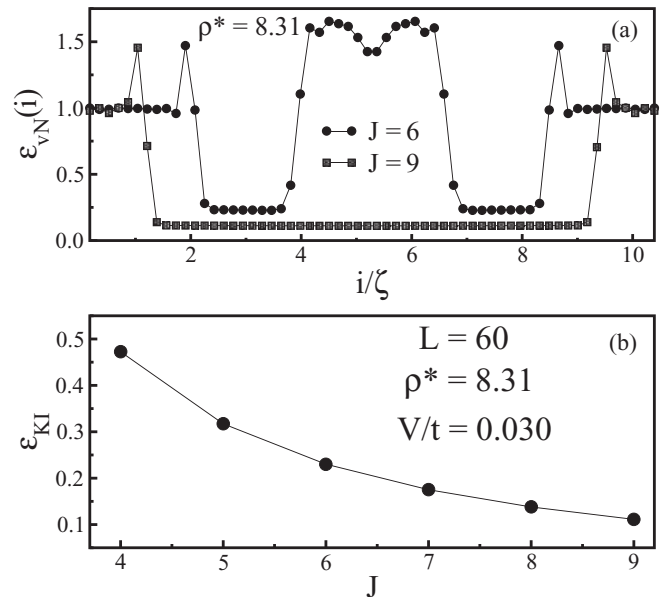

FIG. 4. (a) Local von Neumann entropy for a system with $\rho^* = 8.31$ and two different local couplings $J = 6$ and 9. (b) Local von Neumann entropy at the Kondo insulator domain vs the local coupling for a system with $N = 48$ and $V/t = 0.030$.

the Kondo insulator domain, which increases with the local coupling [compare Figs. 2(f) and 4(a)]. The above behavior is expected, since the delocalized and localized atoms tend to form singlets when the local coupling increases, which causes the atoms to be less confined in the trap; i.e., the atoms are more spread in the lattice trap, as can be seen in Fig. 4(a). Observing Figs. 2(f) and 4(a), we note that the local von Neumann entropy value at the Kondo insulator domain (ε_{KI}) decreases as the local coupling grows. This tendency is shown in Fig. 4(b) for more values of J. This behavior is expected, since as the coupling increases, the system tends to be more orderly and extended in the lattice, which reduces the entanglement. Also, as J takes larger values, the ground-state function can be written as a product of local singlet states more easily, and the entanglement will be smaller.

We expected that the block von Neumann entropy obtained by calculating the reduced density matrix for the half system would provide us with information on the ground state of the Kondo lattice model plus a harmonic potential, in the same way as Silva-Valencia *et al.* [18] and Campostrini *et al.* [19,20] showed that it was useful for describing fermions and bosons confined in one-dimensional optical lattices.

IV. CONCLUSIONS

We studied the link between the entanglement and the ground state of alkaline-earth-metal fermionic atoms confined in harmonic traps, using the density-matrix renormalization group method. We evaluated the local von Neumann entropy

measure of entanglement and found that this quantity varies in the metallic regions, whereas it remains constant in the insulator regions. In the band-insulator regions, the local von Neumann entropy takes the value of 1 because we have only two different states, determined by the orientation of the nuclear spin of the localized atoms. The local von Neumann entropy is <1 at the Kondo insulator domains, and its value decreases with the local coupling, whereas it is almost independent of the confining potential.

Although the ground states considered here are not truly phases in the thermodynamic sense, we show evidence that the local von Neumann entropy, the average entropy, and their derivative are useful tools for studying quantum transitions in impurity systems.

A goal of this paper was to show a one-to-one correspondence between the local von Neumann entropy and the variance of the particle density, which can be used to measure the entanglement in experiments. Recently, Calabrese *et al.* [21] derived exact relations between the Rényi entanglement entropies and the particle-number fluctuations of noninteracting fermions, motivating the search for new ways to experimentally measure the entanglement.

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