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Possible critical behavior driven by the confining potential in optical lattices with ultra-cold fermions

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ABSTRACT

A recent paper [V.L. Campo, et al., Phys. Rev. Lett. 99 (2007) 240403] has proposed a two-parameter scaling method to determine the phase diagram of the fermionic Hubbard model from optical lattice experiments. Motivated by this proposal, we investigate in more detail the behavior of the ground-state energy per site as a function of trap size (L) and confining potential ($V(x) = t(x/L)^\alpha$) in the one-dimensional case. Using the BALDA–DFT method, we find signatures of critical behavior as $\alpha \rightarrow \infty$.

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1. Introduction

The Hubbard model was proposed in the 1960s as a simplified model of a system of correlated fermions, capturing the competition between localisation due to strong interparticle repulsion and itinerant behavior due to intersite hopping. It remains a model of central importance in condensed matter physics; but despite this fact, and decades of investigative effort, the model in dimensions $d > 1$ remains unsolved, and its phase diagram is still a subject of controversy.

Recently, a new line of attack has been proposed [1]: to determine the phase diagram of the Hubbard model not using theory, but using cold-atom experiments which—unlike traditional condensed matter systems—should be essentially perfectly described by the Hubbard Hamiltonian. This is for two reasons. Firstly, the lattice in the cold-atom case is provided by a laser standing wave (or ‘optical lattice’), which can be made almost perfectly periodic and sinusoidal. Secondly, the interaction between the neutral atoms should be well described by a contact interaction of the Hubbard form [2,3]. Other advantages of such experiments include the following: the inter-atomic interaction strength and hopping amplitude in these systems can be tuned over a wide range; the achievable particle numbers are much greater than those available in current computer-based simulations of fermionic systems; and the total energy (for example) is an easily measurable quantity.

However, a major difference between the solid-state and cold-atom realisations of the Hubbard model is the nature of the particles’ confinement. In the solid-state case, it is of the ‘hard-wall’ type, where the system is homogeneous except for a very high potential step at its edges; in the cold-atom case, the confining potential arises from an external electromagnetic field, and is almost always harmonic, leaving no residue of translational invariance. How to extract the phase diagram of the homogeneous model from these inhomogeneous systems is discussed in Ref. [4], where a two-parameter scaling method is proposed, with the two parameters L and α representing respectively the size and shape of the confining potential. The method involves considering different such shapes (i.e. different values of α), and determining for each of them a thermodynamic ($L \rightarrow \infty$) limit of some intensive quantity such as the energy per site. Then one analyzes the dependence of that quantity on the shape of the confining potential and extrapolates (in α) to the homogeneous (‘hard-wall’) limit.

It has been empirically observed [4], at least in the one-dimensional case, that the rate of convergence to the thermodynamic limit is dependent on the shape of the confining potential. Here, we address that question in more detail. In the course of so doing, we find that the behavior during the second extrapolation, i.e. the extrapolation in the shape of the potential towards the homogeneous limit, displays signatures of critical behavior.

2. Model, and previously published results

We consider the following inhomogeneous one-dimensional Hubbard model:

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$$\hat{H} = -t \sum_{j,\sigma} (\hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma} + \text{H.c.}) + U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} + \sum_{j,\sigma} V(x_j) \hat{n}_{j,\sigma}, \quad (1)$$

where $\hat{c}_{j,\sigma}^\dagger$ creates a fermion with z-component of spin σ at site j , t measures the hopping integral between neighboring sites, U is the strength of the local interaction between two fermions of opposite spins, $\hat{n}_{j,\sigma} = \hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma}$ is the number operator for spin σ at site j , and $V(x)$ is the external potential rendering the model inhomogeneous. The position of the site j is $x_j = ja$, where a is the lattice parameter of the chain, and j takes any integer value. The external potential assumes the general form

$$V(x) = t \left| \frac{x}{L} \right|^\alpha, \quad (2)$$

with $\alpha > 0$, and therefore confines the fermions to a region of size $\sim 2L$, or more precisely, makes the probability of finding a fermion at x with $|x| \gg L$ negligible. Accordingly, we refer to $2L$ as the system size, and $2L/a$ as the number of sites, irrespective of the value of α . This allows us to define an intensive quantity as the corresponding extensive quantity divided by $2L/a$. In particular, we will be concerned here with the energy per site, $Ea/2Lt$, and with the filling $f = Na/2L$, where N is the number of fermions.

The above Hubbard model, and its higher dimensional versions, can be realised with trapped ultra-cold fermionic atoms in the presence of an optical lattice with suitable laser intensity and wavelength (see Fig. 1). The atoms are confined by an additional external potential whose exponent α is usually equal to 2. In optical traps with Gaussian laser beams, a suitable superposition of two laser beams could eliminate the harmonic part of the potential, leaving a quartic one. Such trap has already been reported [5]. Similarly, superposing three or more laser beams, one could generate trap potentials with exponents of 6, 8, and so on. Despite the increasing experimental difficulties involved in making traps with higher exponents, the two-parameter scaling method relies on this possibility. For applications to solid-state systems, one would be interested in the thermodynamic limit ($L \rightarrow \infty$) of the above model with $\alpha = \infty$ (a square well potential of width $2L$).

As Fig. 2 illustrates, given a finite exponent in the confining potential, simply increasing the size of the trap, L , is not enough to recover the homogeneous results. Traps with different exponents α have different thermodynamic limits of energy per site, and the same must happen with other properties. The unavoidable confining potential with a finite exponent poses, therefore, an intrinsic obstacle to the extraction of the homogeneous model's

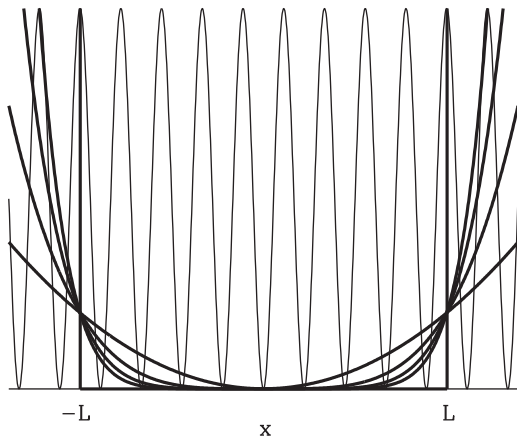


Fig. 1. Optical lattice and different confining potentials. The optical lattice with a high amplitude defines the sites and makes it possible to describe the system by means of a Hubbard model, which is however inhomogeneous due to the confining potential (thick lines). As the exponent α in (2) tends to ∞ , the confining potential approaches the square well shape with width $2L$.

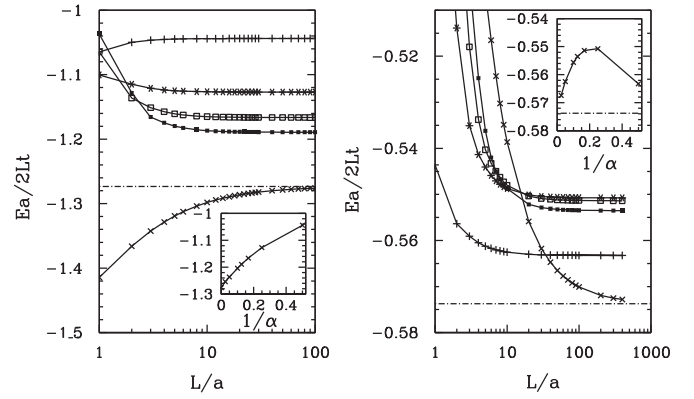


Fig. 2. Dependence of total energy on system size for different trap exponents, $\alpha = 2$ (+), 4 (*), 6 (\square), 8 (\blacksquare) and ∞ (\times). The filling is fixed at $f = 1$. We show results for non-interacting fermions ($U = 0$) on the left and for interacting fermions ($U = 4t$) on the right. Notice that for finite values of α the thermodynamic limit is attained with smaller system sizes than in the $\alpha = \infty$ case. Insets: the same quantity in the thermodynamic limit plotted against α^{-1} . Figure reproduced from Ref. [4].

phase diagram from such experiments. To overcome it, one must make a sequence of experiments [4] with different exponents and then extrapolate the results to get the limit $\alpha \rightarrow \infty$.

3. Method, and new results

In order to achieve a better understanding of the role the trap exponent α plays in the dependence of the energy per site on the system size, we investigate both non-interacting ($U = 0$) and interacting ($U \neq 0$) systems. While the former require only the diagonalization of a tridiagonal matrix, the latter require methods which can deal with the strong correlations coming from the interactions. We choose an approach based on density-functional theory (DFT) [6], which has been specially developed to treat the one-dimensional inhomogeneous Hubbard model [7,8]. Its energy functional is constructed by means of the local density approximation based on the exact Bethe Ansatz solution for the homogeneous model: this approximation is termed BALDA. Comparisons between BALDA and quantum Monte Carlo (QMC) results demonstrate that BALDA gives ground-state energies with an accuracy of a few percent [8].

Our numerical simulations show that as the system size, $2L$, goes to infinity, the system's ground-state energy per site approaches its thermodynamic limit according to

$$\varepsilon(L) = \frac{a}{2L} E(L) = \varepsilon_\infty + \left(\frac{2L}{\xi} \right)^{-\gamma}, \quad (3)$$

where ε_∞ , ξ , and γ all depend on the trap exponent α in a way which resembles critical behavior, with the hard-wall case ($\alpha = \infty$) corresponding to the critical point.

In Fig. 3, we show that the energy per site follows Eq. (3) for both non-interacting and interacting systems. Through the fitting we can extract the dependence of its three parameters on the trap exponent (Fig. 4). Although Fig. 3 only displays results for filling $f = 0.5$, we have found similar behavior for different fillings ($f = 1$ and 1.5) and different interaction strengths ($U = 4t$ and $8t$).

Fig. 4 displays the dependence of the thermodynamic limit of energy per site ε_∞ , the finite-size scaling exponent γ , and the length ξ on the trap exponent α . These graphs are reminiscent of critical behavior, with $\alpha^{-1} = 0$ (i.e. the square-well trap) as the critical point. While the thermodynamic-limit energy ε_∞ is a continuous function of α^{-1} , the exponent γ seems to be discontinuous at $\alpha^{-1} = 0$, and the length ξ seems to diverge as

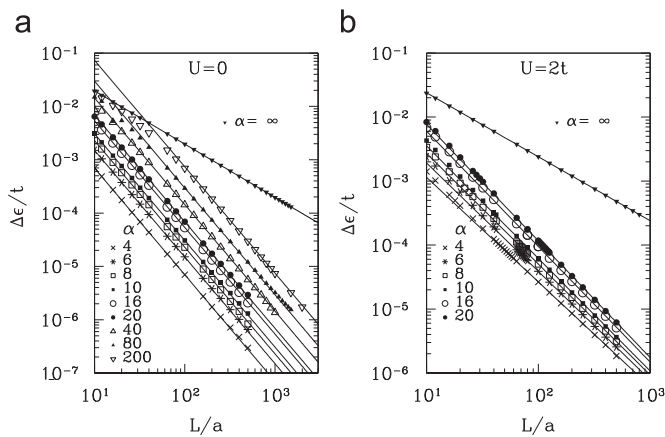


Fig. 3. Dependence of $\Delta\epsilon = E/2L - \epsilon_\infty$ on the system size for (a) non-interacting fermions ($U = 0$) and (b) interacting fermions ($U = 2t$). In both cases, numerical data from systems with filling $f = 0.5$ were used. For each value of the trap exponent, α , Eq. (3) fits the data very well even for quite small systems. Similar behavior is found for fillings $f = 1.0$ and 1.5 and also interaction strengths $U = 4t$ and $8t$.

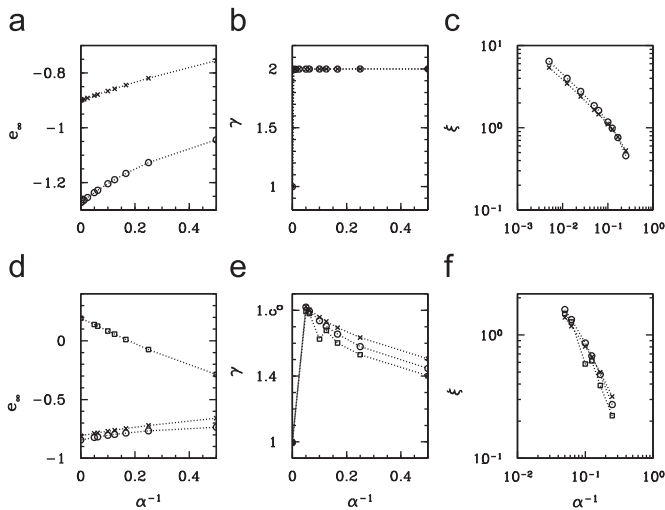


Fig. 4. Dependence of the thermodynamic limit of energy per site, e_∞ , of the finite-size scaling exponent, γ , and of the correlation length, ξ , on the trap exponent, α , for non-interacting ((a)–(c)) and interacting ((d)–(f)) fermions. In the non-interacting case, we show results for fillings $f = 0.5$ (x) and 1.0 (o); in the interacting ($U = 2t$) case, we show in addition results for $f = 1.5$ (◻).

$\alpha^{-1} \rightarrow 0$ —lending support to our use of the term ‘correlation length’.

Note that, in the interacting case, the finite-size scaling exponent γ is α -dependent, and furthermore seems to tend to the non-interacting value $\gamma = 2$ as $\alpha^{-1} \rightarrow 0$. Also, in all finite- α cases we have $\gamma > 1$. This accords with our earlier observation that the thermodynamic limit is more easily achieved for finite trap exponents. The reason for this is likely to be that for finite α the wave functions can extend beyond $|x| = L$. Thus the system does not end abruptly, which in turn avoids strongly perturbing the fermionic fluid.

The apparent discontinuity in $\gamma(\alpha)$ at $\alpha^{-1} = 0$, however, remains surprising. In the non-interacting case, we have performed calculations for α as large as 200. Looking carefully at Fig. 3a, one can see that in the case $\alpha = 200$, the points corresponding to smaller systems seem to follow a line whose γ is equal to 1; but as the system size becomes larger, the energy starts to follow the line with $\gamma = 2$. We can, therefore, identify a

transition length, L_T , and we expect L_T to become larger and larger as the trap exponent is increased, diverging when $\alpha^{-1} \rightarrow 0$. This implies a relation between L_T and the correlation length ξ , though additional computations with larger systems are necessary to determine its nature.

The dependence on filling fraction, f , is also instructive. The finite-size scaling exponent γ and the correlation length ξ do depend on f ; however, the plots indicate that this dependence disappears as we approach the critical point $\alpha^{-1} = 0$. This is exactly what we would expect in a critical scenario: the critical point would be described only by its universality class, which would be independent of a parameter like the filling fraction. In particular, the slopes in Figs. 4c and f are essentially the same for the different fillings and give us directly the critical exponent ν associated to the correlation length. We obtain $\nu \sim 0.51$ for non-interacting fermions and $\nu \sim 0.70$ for interacting fermions. We must emphasise, however, that this latter is a rough estimate only. Computations with larger systems will be necessary to determine the true behavior of interacting fermions near the critical point, even if the BALDA method is reliable in such extreme cases.

4. Conclusions

In conclusion, we have considered the inhomogeneous one-dimensional Hubbard model, studying the evolution of the ground-state energy per site towards its thermodynamic limit as the system size is increased. Looking at the role played by the trap exponent, we have found an apparently critical behavior, which still needs more detailed characterization. While the results for non-interacting fermions are exact, the results for interacting fermions were obtained within the BALDA approximation.

Since the observed critical behavior has a geometrical origin, we expect that such behavior must happen independently of the interaction strength. Our treatment using BALDA can be interpreted as a mean field calculation, which is able to capture the critical behavior but gives inaccurate results for critical exponents, for example. To overcome this methodological limitation, one should adopt more accurate computational methods, such as QMC [9] or density matrix renormalization group (DMRG) [10]. These are, however, much more computationally intensive than a DFT calculation.

From the analytical point of view, even the non-interacting case deserves further exploration. In particular, in the absence of interactions it should be easier to find a renormalization group approach with a convenient decimation scheme to extract the critical behavior accurately. Once such scheme has been found, given the similarity between the interacting and non-interacting results, such an approach could be tentatively generalized to the interacting case.

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