Properties of the $U \gg t$ One-Dimensional Hubbard Model at Half-Filling

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We examine the one-dimensional Hubbard model and derive expressions for the chemical potential and momentum distribution in the limit of strong electron-electron interactions to first order in perturbation theory. By showing that the perturbation matrix is stochastic, the chemical potential is found to depend only on the model parameters and not on the system size, consistent with the well-known result in the thermodynamic limit. The momentum distribution for electrons of a given spin is found to depend only on the fraction of electrons with that spin.

I. INTRODUCTION

The Hubbard model[1,2] represents the electronic properties of molecules and solids in the form of both electron-lattice and electron-electron interaction terms. The competition between these two terms is vital to the understanding of many properties of materials. For example, in the early days of quantum theory it was discovered that the insulating behavior of some solids, like the transition metal oxide NiO, could not be explained by independent electron theories alone.[3,4] Although the Hubbard model oversimplifies these effects by including only nearest-neighbor tight-binding terms and including only electron-electron interactions in the same non-degenerate orbital state, it has enjoyed some success in representing narrow band solids and Mott insulators.

In second quantization, the Hubbard Hamiltonian is[1,2]

$$\begin{aligned}\mathcal{H}(t,U) &= K(t)+V(U) \\ &= -t\sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} \end{aligned} \quad (1)$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) an electron with spin σ in the Wannier state localized at site i, $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$ is the number operator, t is the energy associated with an electron hopping between adjacent sites, U is the on-site Coulomb repulsion energy, and the notation $\langle i,j\rangle$ restricts the sum to over nearest neighbor sites only. We are interested in a one-dimensional lattice consisting of N electrons and N_s lattice sites. Periodic boundary conditions are imposed, giving every site exactly two nearest neighbors.

Much attention has been given to this model in the thermodynamic limit. Using a form of the Bethe ansatz for fermions,[5] Lieb and Wu found an exact expression for the ground state energy as a function of U and found that no Mott transition occurs for $U > 0$.[6] The spectrum of low excited sites has been calculated for both a half-filled band[7] and arbitrary filling,[8,9] as has the magnetic susceptibility.[10] This list is by no means comprehensive.

Finite size systems have also been studied for a variety of small systems, with special emphasis being placed on the case where $N = N_s = 6$ (e.g. the π electron system in a benzene molecule).[11,12] Our interest lies in the ground state properties of these systems in the limit of strong intrasite repulsion ($U \gg t$). These systems have been studied for arbitrary filling,[13] leading to upper and lower bounds on the ground state energy.[14,15] For our present work, we only consider the half-filled case

$$\frac{N}{N_s} = 1. \quad (2)$$

In this case, the ground state favors magnetic moments at each site due to the vanishing probability of doubly occupied sites and, in the thermodynamic limit, has been shown to be an insulator.[6]

We calculate the chemical potential for finite systems of arbitrary size at zero temperature to first order in perturbation theory. Results indicate that for a certain class of systems, which are defined in the next section, the chemical potential of the ground state with strong electron-electron interactions is independent of the size of the chain. In addition, we calculate the momentum distribution and find that it only depends upon the fraction of each spin type. Plots of both quantities as a function of U are given for some small systems to illustrate these behaviors. Numerical results shown in this paper were obtained by exact diagonalization methods.

II. CHEMICAL POTENTIAL

In their study of the Hubbard model in the thermodynamic limit, Lieb and Wu defined *two* chemical potentials corresponding to either the addition (μ_+) or removal (μ_-) of an electron to the ground state. For a fixed number of sites, the chemical potentials (known as the electron affinity and electron ionization potentials, respectively) are defined as[6]

$$\mu_+ = \varepsilon(M+1,U) - \varepsilon(M,U) \quad (3)$$
$$\mu_- = \varepsilon(M,U) - \varepsilon(M-1,U), \quad (4)$$

where $\varepsilon(M,U)$ is the ground state energy associated with M electrons with intrasite repulsion U. For notational convenience, the dependence of the energy on N_σ (the total number of electrons with spin σ) has not been explicitly written. While Eqs. (3) and (4) are valid for an arbitrary number of electrons, Lieb and Wu also showed that for the half-filled case, where $M = N$ from Eq. (2),

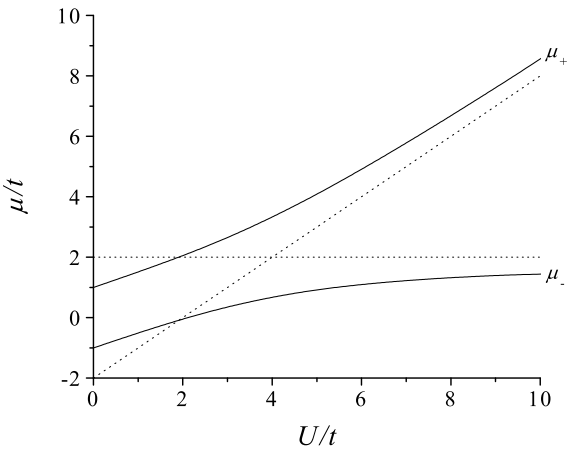

FIG. 1: Plot of the chemical potentials μ_+ and μ_- as a function of U/t for $N_s = 6$ and $N_\sigma = 3$. As U/t increases, these potentials asymptotically approach the dotted lines.

the chemical potentials are related at all U by

$$\mu_+ = U - \mu_-. \tag{5}$$

It is important to note that for a finite system with periodic boundary conditions, the relation given in Eq. (5) is only true if N_s (and therefore, N) is even. In that case, it has been shown that the ground state has spin $S_z = 0$,[16] which implies that

$$N_\sigma = \frac{N}{2}, \quad \sigma = \uparrow, \downarrow \tag{6}$$

where $\sum_\sigma N_\sigma = N$. The spin symmetry described in Eq. (6) makes the spin of the electron being added or removed in Eq. (3) and (4) arbitrary.

In order to study the behavior of μ_+ and μ_- at large U we treat the tight-binding term $K(t)$ as a perturbation. For a system of M electrons, the ground state energy of the unperturbed Hamiltonian $V(U)$ is known

$$V(U)|\alpha^{(0)}(M)\rangle = \varepsilon_\alpha^{(0)}(M)|\alpha^{(0)}(M)\rangle, \tag{7}$$

and d-fold degenerate

$$\varepsilon_1^{(0)}(M) = \ldots = \varepsilon_d^{(0)}(M) \equiv \varepsilon^{(0)}(M). \tag{8}$$

As long as $M \leq N_s$, the unperturbed ground state energy is necessarily zero, $\varepsilon^{(0)}(M) = 0$, and the level of degeneracy is

$$d = \frac{N_s!}{(N_s - M)!M_\uparrow!\, M_\downarrow!}. \tag{9}$$

The first order correction to the ground state energy can be found by diagonalizing the tight-binding Hamiltonian $K(t)$ with respect to the unperturbed ground states $|\alpha^{(0)}(M)\rangle$ and $|\beta^{(0)}(M)\rangle$

$$\begin{aligned}\langle\alpha^{(0)}(M)|K(t)|\beta^{(0)}(M)\rangle & \\ = \; -2t\langle\alpha^{(0)}(M)|K(-\tfrac{1}{2})|\beta^{(0)}(M)\rangle.&\end{aligned} \tag{10}$$

If $M = N$, $K(t)|\beta^{(0)}(N)\rangle$ only contains terms with exactly one doubly occupied site, so

$$\langle\alpha^{(0)}(N)|K(t)|\beta^{(0)}(N)\rangle = 0. \tag{11}$$

Therefore, the first order correction is also d-fold degenerate and zero, independent of our choice of N_σ. Assuming that N_σ satisfies Eq. (6) we conclude to first order in perturbation theory that

$$\lim_{U\to\infty} \varepsilon(N, U) = 0. \tag{12}$$

We now must find the first order correction for a system of $N - 1$ electrons. Due to the degeneracy of the unperturbed ground state, the states described in Eq. (7) are not uniquely defined; any linear combination of these unperturbed states will produce a new state with the same energy. Therefore, we are given some control and choose as our unperturbed $N - 1$ electron states

$$|\alpha^{(0)}(N-1)\rangle = \left(\prod_{i\neq j}{}' c^\dagger_{i,\sigma_i}\right)|0\rangle \;\text{ with }\; \sum_i \sigma_i = \frac{\hbar}{2}, \tag{13}$$

where the index α denotes one possible choice of site index j and spin configuration. The notation $\prod'$ means that the product is only over the variable i, with $i \neq j$. The number of degenerate states is given by Eq. (9). We have chosen the spin of the removed electron to be $-\hbar/2$ which is reflected in the spin constraint in Eq. (13). The result does not depend on this choice.

The correction energy is simply the smallest eigenvalue of the matrix defined in Eq. (11), which can be found by using the largest eigenvalue of the dimensionless matrix $K(-\frac{1}{2})$. Since every site has exactly two nearest neighbors, and each of our unperturbed states have only one vacant site for an electron to move to, each row and column of $K(-\frac{1}{2})$ has only two nonzero elements which, for $N > 2$, are either $\pm\frac{1}{2}$. Furthermore, since $N - 1$ is odd, it is easy to show that

$$\langle\alpha^{(0)}(N-1)|K(-\tfrac{1}{2})|\beta^{(0)}(N-1)\rangle \geq 0, \tag{14}$$

which forces the nonzero elements to be $\frac{1}{2}$. Therefore, the sum of the elements in every row or column is 1

$$\sum_\alpha \langle\alpha^{(0)}(N-1)|K(-\tfrac{1}{2})|\beta^{(0)}(N-1)\rangle = 1 \tag{15}$$

and

$$\sum_\beta \langle\alpha^{(0)}(N-1)|K(-\tfrac{1}{2})|\beta^{(0)}(N-1)\rangle = 1. \tag{16}$$

Matrices that satisfy Eq. (14) and either Eqs. (15) or (16) are well studied and are known as stochastic (since $K(-\frac{1}{2})$ satisfies both, it is *doubly stochastic*). These matrices describe the transitions of a Markov chain; their elements are the transition probabilities that a system will jump from one state to another. Eqs. (15) or (16) state

that the total probability of transition is unity. By identifying that the first order correction matrix is stochastic, we are able to make use of a very important property of all such matrices: their maximum eigenvalue is 1.[17] Therefore, to first order in perturbation theory

$$\lim_{U\to\infty} \varepsilon(N-1,U) = -2t, \tag{17}$$

so that

$$\lim_{U\to\infty} \mu_+ = U - 2t \tag{18}$$

$$\lim_{U\to\infty} \mu_- = 2t. \tag{19}$$

The energy gap between these potentials is simply

$$\lim_{U\to\infty} (\mu_+ - \mu_-) = U - 4t. \tag{20}$$

Therefore, as U increases, μ_+ and μ_- tend toward values which are independent of N_s. The asymptotic behavior of these potentials is shown in Figure 1 for $N = 6$. A similar behavior has been seen in other systems.

In the thermodynamic limit, μ_- was found to be[6]

$$\mu_- = 2t - 4t\int_0^\infty \frac{J_1(\omega)d\omega}{\omega\left[1+\exp\left(\frac{\omega U}{2t}\right)\right]}, \tag{21}$$

where J_1 is a first order Bessel function of the first kind. As $U \to \infty$, the second term in Eq. (21) vanishes and we are left with the same result as Eq. (19).

III. MOMENTUM DISTRIBUTION

In this section we again consider $U \gg t$ and assume the half-filling condition described in Eq. (2), though N_s need not be even. No condition is placed on the spin number operator N_σ. We are interested in finding the momentum distribution of the lowest energy state with respect to a given spin configuration, $|\psi\rangle$. The expectation value of the tight-binding portion of the Hubbard Hamiltonian is given by

$$\langle\psi|K(t)|\psi\rangle = -2t\sum_{k\sigma}\cos(ka)\,\tilde{n}_{k\sigma} \tag{22}$$

where a is the lattice constant and $\tilde{n}_{k\sigma}$ is the momentum distribution

$$\tilde{n}_{k\sigma} = \langle\psi|\tilde{c}^\dagger_{k\sigma}\tilde{c}_{k\sigma}|\psi\rangle, \tag{23}$$

which counts the number of electrons with spin σ and momentum k. Taking the Fourier transform

$$\tilde{c}_{k\sigma} = \frac{1}{\sqrt{N_s}}\sum_j e^{ikja}c_{j\sigma} \tag{24}$$

yields an expression for $\tilde{n}_{k\sigma}$ in the site-spin representation

$$\tilde{n}_{k\sigma} = \frac{1}{N_s}\sum_{j\ell} e^{ika(j-\ell)}\gamma^{j\sigma}_{\ell\sigma}, \tag{25}$$

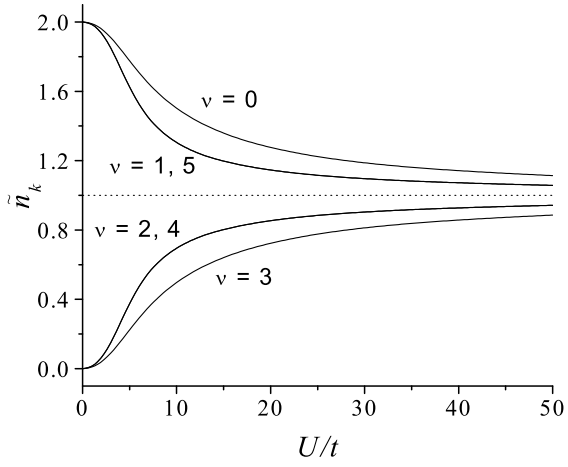

FIG. 2: Plot of the spin-independent momentum distribution $\tilde{n}_k$ as a function of U/t for $N_s = 6$ and $N_\sigma = 3$. As U/t increases in strength, the occupancy of each k-value asymptotically approaches 1 (dotted line).

where j is an integer and we introduced the one-particle reduced density matrix

$$\gamma^{j\sigma}_{\ell\sigma} = \langle\psi|c^\dagger_{j\sigma}c_{\ell\sigma}|\psi\rangle. \tag{26}$$

For periodic boundary conditions, ka takes discrete values indexed by ν

$$ka = \frac{2\pi\nu}{N_s},\ \ \nu = 0,1,...,N_s-1. \tag{27}$$

Using the Hermiticity and trace of γ

$$\sum_i \gamma^{i\sigma}_{i\sigma} = N_\sigma, \tag{28}$$

$\tilde{\mathrm{n}}_{k\sigma}$ can be rewritten as

$$\tilde{n}_{k\sigma} = \frac{1}{N_s}\left\{\sum_{j\neq\ell}\cos\left(\frac{2\pi\nu(j-\ell)}{N_s}\right)\gamma^{j\sigma}_{\ell\sigma} + N_\sigma\right\}. \tag{29}$$

When $U = 0$, the occupancy of each allowed k-value can be trivially found by minimizing Eq. (22) with respect to $\tilde{n}_{k\sigma}$. We are interested in the nature of this distribution when $U \gg t$. In this limit, the expectation of any site to be doubly occupied vanishes, so the lowest energy state has only one electron per site. This, along with the translational symmetry of our chain, means that

$$\lim_{U\to\infty}\gamma^{i\sigma}_{j\sigma} = \frac{N_\sigma}{N_s}\delta_{i,j} \tag{30}$$

which forces Eq. (29) to become k-independent

$$\lim_{U\to\infty}\tilde{n}_{k\sigma} = \frac{N_\sigma}{N_s}\ ,\ \forall\, k. \tag{31}$$

Therefore, in the case of strong coupling, the momentum distribution becomes uniform. In Figure 2, the momentum distribution is plotted as a function of U for a spin

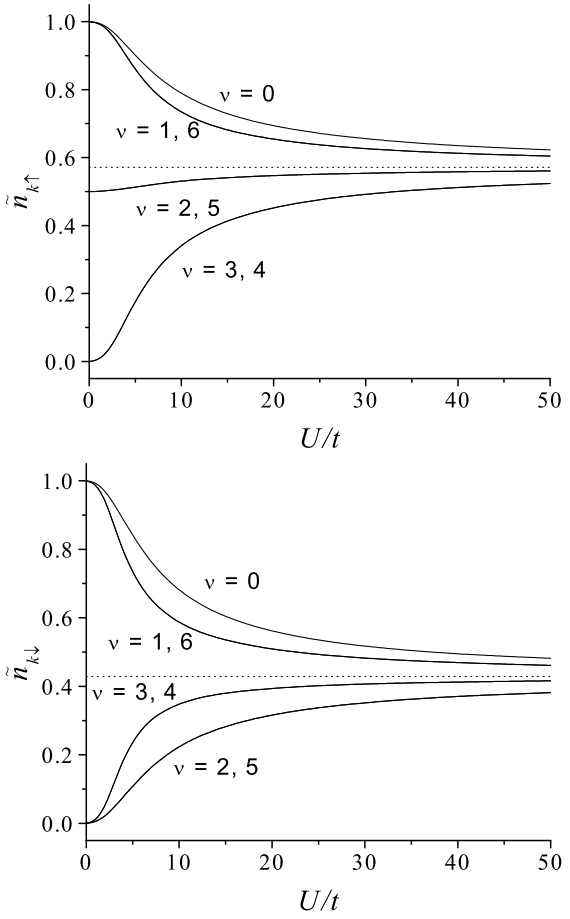

FIG. 3: Plots of the momentum distribution (*top*) $\tilde{n}_{k\uparrow}$ and (*bottom*) $\tilde{n}_{k\downarrow}$ for $N_s = 7$ with $N_\uparrow = 4$ and $N_\downarrow = 3$. As U/t increases, $\tilde{n}_{k\sigma}$ approaches N_σ/N_s (dotted line).

symmetric ground state with $N = 6$. Due to the spin symmetry, $\tilde{n}_{k\uparrow} = \tilde{n}_{k\downarrow}$, so the spin-independent momentum distribution $\tilde{n}_k = \sum_\sigma \tilde{n}_{k\sigma}$ is shown instead. However, unlike the results for the chemical potential, Eq. (31) is true for the lowest energy state of any half-filled system characterized by a given spin configuration N_σ. Figure 3 shows an example with $N = 7$, $N_\uparrow = 4$ and $N_\downarrow = 3$. These results are consistent with previous work done on the spin independent momentum distribution of the ground state at large U.[18]

IV. SUMMARY

The chemical potential and momentum distribution of the ground state of a half-filled Hubbard chain were calculated in the limit of strong electron-electron interactions. We showed that these properties exhibit asymptotic behavior in this limit, independent of the size of the system. Results were found by treating the hopping term as a perturbation, with calculations taken to first order.

The electron affinity and ionization potentials were found to approach values independent of the size of the system. A maximal energy gap between these potentials was found to be $U - 4t$. These finite size results agree with work done by Lieb and Wu in the thermodynamic limit. Likewise, the momentum distribution was found to exhibit asymptotic behavior independent of the system size, though it is dependent upon the fraction of each spin type. Plots of both the chemical potentials as well as the momentum distribution were given for several small systems as a function of U/t.

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[1] J. Hubbard, Proc. Roy. Soc. A **276**, 238 (1963).
[2] J. Hubbard, Proc. Roy. Soc. A **277**, 237 (1964).
[3] J. H. de Boer and E. J. W. Verwey, Proc. Phys. Soc. **49 (4S)**, 59 (1937).
[4] N. F. Mott and R. Peierls, Proc. Phys. Soc. **49 (4S)**, 72 (1937).
[5] C. N. Yang, Phys. Rev. Lett. **19**, 1312 (1967).
[6] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[7] A. A. Ovchinnikov, Zh. Eksp. Teor. Fiz. **57**, 2137 (1969), [Sov. Phys. JETP **30**, 1160 (1970)].
[8] C. F. Coll III, Phys. Rev. B **9**, 2150 (1974).
[9] F. Woynarovich, J. Phys. C: Solid State Phys. **15**, 85 (1982).
[10] H. Shiba, Phys. Rev. B **6**, 930 (1972).
[11] O. J. Heilmann and E. H. Lieb, Trans. N.Y. Acad. Sci. **33**, 116 (1970).
[12] M. Nauciel-Bloch and T. P. Eggarter, Phys. Rev. A **19**, 1862 (1979).
[13] J. Oitmaa, Y. Jie, J. A. Henderson, and Z. Weihong, Phys. Rev. B **48**, 6210 (1993).
[14] S. A. Trugman, Phys. Rev. B **42**, 6612 (1990).
[15] F. Becca, L. Capriotti, S. Sorella, and A. Parola, Phys. Rev. B **62**, 15277 (2000).
[16] E. Lieb and D. Mattis, Phys. Rev **125**, 164 (1962).
[17] A. Berman and R. J. Plemmons, *Nonnegative Matrices in the Mathematical Sciences* (Academic Press, Inc., New York, USA, 1979).
[18] M. Takahashi, J. Phys. C: Solid State Phys. **10**, 1289 (1977).