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EXPONENTS FOR ONE DIMENSIONAL LARGE U
HUBBARD MODEL IN THERMODYNAMIC LIMIT

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**MOMENTUM DISTRIBUTION CRITICAL EXPONENTS
FOR ONE DIMENSIONAL LARGE U HUBBARD MODEL
IN THERMODYNAMIC LIMIT¹**

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ABSTRACT

The critical exponents of the momentum distribution near k_F , $3k_F$ and $5k_F$ are studied numerically for one-dimensional $U \rightarrow \infty$ Hubbard model, using finite size systems and extrapolating them to the thermodynamic limit. Results at k_F agree with earlier calculations, while at $3k_F$, exponents less than 1 are obtained for finite size systems with extrapolation to 1 (regular behavior) in the thermodynamic limit, in contrast to earlier analytic prediction $9/8$. The distribution is regular at $5k_F$ even for finite systems. The singularity near $3k_F$ is interpreted as due to low energy excitations near $3k_F$ in finite systems.

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Since the realization that electron-electron correlations play an important role in strongly correlated systems, the Hubbard model has attracted a lot of attention. Related to many strongly correlated systems [1], one-dimensional (1D) Hubbard model serves as a prototype to get the basic understanding and to elucidate the main concepts for the field. It has a non-Fermi liquid ground state, and the Fermi distribution function does not have a finite jump, but rather a power law singularity at the Fermi surface. Using the large U limit of the Bethe Ansatz solution of the Hubbard model [2], Ogata and Shiba [3] pioneered an explicit numerical calculation of the singularity exponents for various correlation functions. Soon afterwards, the exponent of the spin correlation function was calculated analytically [4], and all the exponents were derived by the bosonization technique [5,6] and mapping onto a conformal field theory [7], based on the Bethe Ansatz solution [2] and the Luttinger liquid framework, proposed by Haldane [8] in the early 80s. These exponents have also been reproduced by a “mean-field” type calculation using non-Abelian gauge transformations [9]. In particular, for the large U limit, an exponent of $1/8$ for the momentum distribution (MD) function at k_F was predicted which has been verified at the same time by numerical calculations [3,10], and later exactly derived for a lattice model in the $U \rightarrow \infty$ limit [11] without resorting to any linear spectrum assumption. A singularity of power $9/8$ at large U has also been predicted to show up at $k = 3k_F$, and a weaker singularity is expected at the $5k_F$ points, too. However, the only available numerical calculation of the $3k_F$ exponent [12] disproves this prediction by showing a $3/4$ exponent for a small size system. Since the previous work [12] on the exponent at $3k_F$ was limited to filling $\nu = 1/4$ and the chain length was only up to $L = 24$, one may suspect that the difference is due to the finite size effect or a special filling. To clarify this issue, a study of critical exponents for longer chains of various fillings has been carried out.

In this paper, the MD $n(k)$ is calculated, following the way designed by Ogata and Shiba [3], and then the critical exponents for $n(k)$ at k_F , $3k_F$, and $5k_F$ points are extracted. This method of calculating $n(k)$ has been developed by these authors into an efficient and very precise technique [4,13,14]. For $N_\uparrow = N_\downarrow$ up to 14, we have calculated $n(k)$ for fillings $\nu = 2/7, 3/7, 1/6, 1/5, 2/5, 1/4, 1/3$ with the corresponding largest chain length 49, 28,

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84, 70, 35, 56, 42, respectively. By a log-log plot [3] for $n(k)$ and k near $5k_F$, no singularity has been found for all finite size systems studied. Hence, no singularity at $5k_F$ point for systems in the thermodynamic limit, either. On the contrary, for $3k_F$ and k_F points, the singularities of MD are evident for any finite size system we have studied. By a more elaborate analysis of $n(k)$, we show that the exponents are $1/8$ for the k_F point and 1 for $3k_F$ in the thermodynamic limit. In the following, we will first give a brief introduction to the method proposed by Ogata and Shiba [3], calculate the exponents for MD, and then discuss the new behavior found for the $3k_F$ point.

The Hubbard model Hamiltonian is:

$$H = -t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}^\dagger$ creates an electron of spin σ at site i . We study the ground state of a system with chain length L , total number of electrons $N = N_\uparrow + N_\downarrow$ and $N_\uparrow = N_\downarrow$. The filling of the system is $\nu = N_\uparrow/L = N_\downarrow/L$. In the $U \rightarrow \infty$ limit, the ground state is a product $|\Psi\rangle \otimes |\Phi\rangle$ in which the charge part $|\Psi\rangle$ is the ground state for N spinless fermion on a chain of length L and the spin part $|\Phi\rangle$ is the ground state of a Heisenberg spin $s = \frac{1}{2}$ chain of length N [3]. To evaluate the MD

$$n(k) = \frac{1}{L} \sum_{i,j} \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle e^{ik(i-j)}, \quad (2)$$

the charge and spin parts are calculated separately [4,13]:

$$\begin{aligned} \langle c_{0\uparrow}^\dagger c_{j\uparrow} \rangle &= \sum_q \langle \Psi | c_{0\uparrow}^\dagger c_j e^{-iq \sum_{i=1}^{j-1} n_i} | \Psi \rangle \\ &\quad \cdot \frac{1}{N} \sum_{r=0}^{N-1} \frac{1}{2} e^{iqr} \langle \Phi | \prod_{m=0}^{r-1} (2\mathbf{S}_m \cdot \mathbf{S}_{m+1} + \frac{1}{2}) | \Phi \rangle, \end{aligned} \quad (3)$$

where $q \frac{N}{2\pi} = 0, \dots, N-1$. We evaluate the charge part in the above equation by its reduced form:

$$\langle \Psi | c_{0\uparrow}^\dagger c_j e^{-iq \sum_{l=1}^{j-1} n_l} | \Psi \rangle = \delta_{0j} - \begin{vmatrix} \delta_{0j} & \psi_1(j) & \dots & \psi_N(j) \\ \psi_1^*(0) & \dots & \dots & \dots \\ \vdots & & \langle \psi_n | \tilde{\psi}_m \rangle & \vdots \\ \psi_N^*(0) & \dots & \dots & \dots \end{vmatrix} \quad (4)$$

$$\begin{aligned} \text{with } \psi_n(r) &= \frac{1}{\sqrt{L}} e^{ik_n r}, \\ \tilde{\psi}_n(r) &= \begin{cases} \psi_n(r), & r = 0 \text{ or } r \geq j \\ e^{-iq} \psi_n(r), & 0 < r < j \end{cases}, \\ k_i &= \frac{2\pi}{L} i - \frac{N+1}{L} \pi, \quad i = 1, \dots, N. \end{aligned}$$

This is a well behaved determinant. We can always reduce the relative error to 10^{-16} in getting its eigenvalues by diagonalization, and the numerical error in calculating the magnitude of this determinant is also negligible. The spin part $\frac{1}{2} \langle \Phi | \prod_{m=0}^{r-1} (2\mathbf{S}_m \cdot \mathbf{S}_{m+1} + \frac{1}{2}) | \Phi \rangle$ is calculated in the exact ground state $|\Phi\rangle$ for the Heisenberg $s = \frac{1}{2}$ chain. We use the reduced density matrix in the configuration space spanned by sites $\mathbf{S}_0, \dots, \mathbf{S}_r$ to evaluate it. Since $\frac{1}{2} \prod_{m=0}^{r-1} (2\mathbf{S}_m \cdot \mathbf{S}_{m+1} + \frac{1}{2})$ has no large eigenvalues compared to the final magnitude (of order 0.1), we do not expect big error appearing in this step, either. Therefore, using this method, we can get high precision result for $n(k)$ of 1D large U Hubbard model.

In Fig.1, we plot $n(k)$ near half filling, namely, $\nu = 5/11$ and $6/11$, which are typical in the range $1/3 < \nu < 2/3$. In Fig.2, we plot $n(k)$ for fillings $\nu = 1/4$ and $3/4$ which are typical for ranges $\nu < 1/3$ and $\nu > 2/3$, respectively. The k_F and $3k_F$ singularities are apparent. Fig.1 and Fig.2 are plotted for finite size systems and they give qualitatively the same $n(k)$ in the thermodynamic limit except near the two singularities (k_F and $3k_F$). From the plot for $n(k)$, we have not observed any weak singularity for $5k_F$. With $n(k)$ for different chain lengths at filling $\nu = 1/6$, following Ogata and Shiba [3], we determine the exponent a_5 for $5k_F$ by [15]

$$n(k) = n_{5k_F} - C_5 |k - 5k_F|^{a_5} \text{sign}(k - 5k_F). \quad (5)$$

To eliminate the numerical error introduced by arbitrariness in choosing n_{5k_F} , we use the

two k points nearest to $5k_F$ ($5k_F + \frac{\pi}{L}$ and $5k_F - \frac{\pi}{L}$ for each L) and find

$$n(5k_F - \pi/L) - n(5k_F + \pi/L) = C_5 \left(\frac{\pi}{L}\right)^{a_5}. \quad (6)$$

Now we plot in Fig.3 $\ln(n(5k_F - \frac{\pi}{L}) - n(5k_F + \frac{\pi}{L})) - \ln(n(5k_F - \frac{\pi}{L_{max}}) - n(5k_F + \frac{\pi}{L_{max}}))$ versus $\ln(\frac{\pi}{L}) - \ln(\frac{\pi}{L_{max}})$ with $L_{max} = 84$. The tangent of the line in the plot is therefore the exponent a_5 . We see the exponent $a_5 = 1$ evidently in Fig.3. Since for all system sizes we have studied the magnitude for a_5 is the same as in Fig.3, the extrapolation ($L \rightarrow \infty$) to the thermodynamic limit does not change this exponent.

In Fig.4, we show the exponents for $3k_F$ and k_F . Using $n(k)$ for fillings $\nu = 2/7, 3/7, 1/6, 1/5, 2/5, 1/4, 1/3$ with the corresponding largest chain lengths 49, 28, 84, 70, 35, 56, 42, respectively, we determine the corresponding exponents. First we remove the arbitrariness in choosing n_{3k_F} and n_{k_F} by writing down equations similar to Eq.(6). Then the exponents a_1 and a_3 in [15]

$$\begin{aligned} n(k) &= n_{3k_F} - C_3 |k - 3k_F|^{a_3} \text{sign}(k - 3k_F), \\ n(k) &= n_{k_F} - C_1 |k - k_F|^{a_1} \text{sign}(k - k_F), \end{aligned} \quad (7)$$

can be written for each pair of successive chain lengths L and $L + \Delta$ at a given filling ν as

$$\begin{aligned} a_3 &= \ln \left(\frac{n(3k_F - \frac{\pi}{L+\Delta}) - n(3k_F + \frac{\pi}{L+\Delta})}{n(3k_F - \frac{\pi}{L}) - n(3k_F + \frac{\pi}{L})} \right) / \ln \left(\frac{\pi/L}{\pi/(L+\Delta)} \right), \\ a_1 &= \ln \left(\frac{n(k_F - \frac{\pi}{L+\Delta}) - n(k_F + \frac{\pi}{L+\Delta})}{n(k_F - \frac{\pi}{L}) - n(k_F + \frac{\pi}{L})} \right) / \ln \left(\frac{\pi/L}{\pi/(L+\Delta)} \right). \end{aligned} \quad (8)$$

By plotting in Fig.4 a_3 and a_1 versus $2/(\ln(\frac{\pi}{L}) + \ln(\frac{\pi}{L+\Delta}))$, we see that the exponents $a_3 = 1$ for $3k_F$ and $a_1 = 1/8$ for k_F in extrapolating $1/\ln(\frac{\pi}{L}) \rightarrow 0$ in the thermodynamic limit. Such an elaborate analysis also provides an explanation why Ogata and Shiba [3] obtained $a_1 = 0.14$ at k_F for finite size systems up to $L = 32$ and why Qin *et al.* [12] found $a_3 = 0.75$ at $3k_F$ for finite size systems up to $L = 24$. Here we have shown $a_3 < 1$ for any finite size systems. However, in the thermodynamic limit, the exponent for $3k_F$ is 1 and the MD shows no singularity at all at that point.

To check the reliability of the $n(k)$ near singularities calculated by the density matrix renormalization group method (DMRG) [16], which is the technique used in studying finite

U Hubbard chain [12], we have compared the absolute values of $n(k)$ calculated by Ogata-Shiba method and DMRG. In Table.1, we list out $n(k)$ at $3k_F \pm \frac{\pi}{L}$ for $\nu = 1/4$ with chain length up to $L = 24$ calculated using the Ogata-Shiba method. Simultaneously, the same MD (denoted by $\hat{n}(k)$ in Table.1) calculated for the same filling and length but finite U ($U = 10^3$) using the density matrix renormalization group (DMRG) technique [12] is also listed. We find these two sets of data differ only in the third digit, and the precision of MD near $3k_F$ in the DMRG calculation is as accurate as for other points.

Now we discuss the physical content of the results obtained. A $n(k)$ exponent smaller than 1 suggests the presence of zero energy quasiparticles in large U , finite size Hubbard chains. Since both k_F and $3k_F$ points have exponents smaller than 1 for finite size systems, certain kind of zero energy quasiparticles of momentum $3k_F$, like those near k_F , are more favorable than other excitations. Previous theoretical prediction for the $3k_F$ exponent was $a_3 \sim 9/8$ by finite size scaling for large, but finite systems [7]. It is quite obvious that exponents greater than 1 cannot be detected in numerical studies like the one we conduct in this paper [17]. Since the theoretical value is greater than one, it cannot provide any explanation for the low energy excitations needed to account for our results. So what was missing in earlier studies?

The linear energy dispersion near the Fermi surface is an essential assumption in both bosonization and conformal field theory treatments [5-7]. As pointed out by Haldane [8], and re-emphasized recently by Schulz [5], the deviation from linear dispersion in actual lattice models should give rise to high harmonics $(2n+1)k_F$, for any integer n , in the fermion operator expansion. This, in turn, may modify the exponents at $3k_F$. However, it seems to be a difficult task to deal with the dispersion $\cos(k)$ exactly and the effect is rather subtle. In fact, the exponent $a_1 = 1/8$ at k_F was calculated without assuming the linear dispersion, based on the phase shift analysis [6,11]. If we generalize that method to $3k_F$, where the phase shift [18] turns out to be $\delta = 3\pi/4$, the exponent $a_3 = \frac{2\delta^2}{\pi^2} = 9/8$ is again obtained. In studies without assuming a linearized spectrum [6,11], only the phase shift of the charge part is used, which, in turn, is affected by excitations of the spin part (see [18] and references therein). So at $3k_F$, the spin effects beyond the phase shift generation should be included to

give an actual explanation. This understanding is supported by the first order perturbation analysis in the small U limit (see Appendix of [3]). In that calculation, the contributions of the $k \sim 2k_F$ excitations of the opposite spin are dominant in $n(k)$ near $3k_F$. In the large U limit, the $3k_F$ singularity shows itself as $k_{F\uparrow} + 2k_{F\downarrow}$ and $k_{F\downarrow} + 2k_{F\uparrow}$ combinations for spin up and spin down electrons, respectively [14]. Anyway, some further studies are certainly needed to clarify the issue.

Comparing a_3 with the well understood exponent $1/8$ for the k_F point, which is due to the zero energy quasiparticle weight suppressed by the orthogonal catastrophe effect [6,11], the behavior $3k_F$ is new, since the zero energy excitation in finite size systems loses its trace in the thermodynamic limit for 1D Hubbard model. At present we do not have a good reason for choosing $1/\ln L$ as scaling variable in Fig.4, and accept it as an “empirical” fact. Probably, a better understanding of low energy excitations in finite systems will provide some justification for it. A similar effect may reappear in the 2D case [1] or shed light on other related problems. If, indeed, this is the case, our numerical results indicate that there is some new physics to be explored.

In summary, we have calculated the MD with its critical exponents at k_F , $3k_F$, and $5k_F$ for $U \rightarrow \infty$ finite systems and have considered the extrapolation to the thermodynamic limit. The calculated power for the MD singularity at k_F agrees with the results of analytical analysis. The calculated power for the MD at $5k_F$ is trivially 1 and indicates there is no singularity near that point at all. However, the calculated exponent for the MD at $3k_F$ is less than one for finite systems, and this singularity diminishes (degenerating into a smooth curve) in the thermodynamic limit. This result disagrees with the analytic prediction $9/8$. We point out that an exponent greater than 1 is not observable numerically, and propose that the effective exponent for $n(k)$ at $3k_F$ is due to a new kind of excitations for finite size systems. This new property at $3k_F$ may lead to a better understanding of this typical non-Fermi liquid. This problem should be investigated further to explore the physics involved.

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[17] Except for the mentioning in [14] that this exponent is around 1 in the absence of magnetic field, while it is bigger than 9/8 for one spin orientation and smaller than 1 for another orientation in the presence of a magnetic field. However, there is always a term of exponent 1 in the expansion of $n(k)$, and this term comes from the incoherent spectrum weight. Since $3k_F$ is not a symmetry point like $k = 0$ or $k = \pi$, we have no reason to find a vanishing coefficient for the exponent 1 term.

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TABLE I. The $n(k)$ around $3k_F$ singularity, at filling $\nu = 1/4$. $n(k)$ is for $U \rightarrow \infty$ calculated by Ogata & Shiba's method [3]. $\tilde{n}(k)$ is for $U = 10^3$ calculated by DMRG [12].

L	8	12	16	20	24
$n(3k_F - \pi/L)$	0.09576	0.08433	0.07790	0.07374	0.07081
$\tilde{n}(3k_F - \pi/L)$	0.09518	0.08384	0.07749	0.07337	0.07048
$n(3k_F + \pi/L)$	0.02663	0.03098	0.03410	0.03641	0.03818
$\tilde{n}(3k_F + \pi/L)$	0.02652	0.03085	0.03398	0.03629	0.03806

FIGURES

FIG. 1. The momentum distribution $n(k)$ for the Hubbard chain near half filling is shown for $\nu = 5/11, 6/11$ for different chain lengths. The zero line of $n(k)$ for $\nu = 6/11$ is shifted to 1. Two singularities at k_F and $3k_F$ are obvious.

FIG. 2. The momentum distribution $n(k)$ for the Hubbard chain far away from half filling is illustrated by $\nu = 1/4, 3/4$ for different lengths. The zero line of $n(k)$ for $\nu = 3/4$ is shifted to 1. Two singularities at k_F and $3k_F$ are evident.

FIG. 3. The leading power of $n(k)$ at $5k_F$ is displayed. The data points plotted are for filling $\nu = 1/6$, with system size $L = 12, 18, \dots, 78$ and $L_{max} = 84$. The fitting line is of slope $a_5 = 1$.

FIG. 4. The exponents a_3 and a_1 for $3k_F$ and k_F (Eq.(7)) are plotted v.s. $2/(\ln(\frac{\pi}{L}) + \ln(\frac{\pi}{L+\Delta}))$. Curves for various fillings ν are shown to yield $a_3 = 1$ and $a_1 = 1/8$ in the thermodynamic limit ($1/\ln(\pi/L) \rightarrow 0$).

Fig.1

Fig.2

Fig.3

Fig.4