Momentum Distribution Critical Exponents for 1D Hubbard model in a Magnetic Field

Nelson O. Nenuwe and John O.A. Idiodi

Department of Physics, Federal University of Petroleum Resources, P.M.B 1221, Effurun, Delta State, Nigeria.

Phone number:+2348037295834,
E-mail of the corresponding author: nenuwe.nelson@fupre.edu.ng

Department of Physics, University of Benin, P.M.B. 1154, Benin City, Edo State, Nigeria

Abstract

Critical exponents at $k_F$, $3k_F$, $5k_F$ and $7k_F$ for the momentum distribution function are studied for one-dimensional Hubbard model in the presence of magnetic field, using conformal field theory (CFT) approach. Exponents at $k_F$ and $3k_F$ are reproduced. Results at $5k_F$ is in contrast to earlier numerical prediction of 1, while at $7k_F$, the exponent is $49/8$. The singularities at $5k_F$ and $7k_F$ appears to be weak and gradually degenerating into a smooth curve.

Keywords

Critical exponent, singularity, momentum distribution.

Academic Discipline

Condensed Matter Physics.

Subject Classification

Theoretical Physics.
1.0 Introduction

Despite one-dimensional (1D) Hubbard model (HM) is the simplest strongly correlated model used to describe the physics of correlated electron systems, the understanding of this model is not complete. This is why calculation of asymptotic correlation functions, momentum distribution (MD) and its critical exponents have not been properly resolved around odd Fermi points. In particular, critical exponents at $3k_F$, obtained by Shaojin et al. [1, 2] disagrees with Ogata and Shiba [3, 4]. The ground state of the 1D HM is a Tomonaga-Luttinger (TL) liquid and the MD function does not show sharp jump, but rather a power-law singularity near the Fermi surface [5]. Ogata and Shiba carried out numerical calculations for critical exponents of MD near $k_F$ and $3k_F$, and obtained 1/8 and 9/8. Soon after, these critical exponents were reproduced analytically [6, 7]. Thereafter, Shaojin et al. [1, 2] carried out Density Matrix Renormalization Group numerical calculations and found that a power-law singularity shows up at $3k_F$ with critical exponent 3/4, and 1 at $5k_F$. The result of Shaojin et al. disagrees with Ogata and others [3-7] at $3k_F$.

We have in this work extended the calculation of critical exponents which has only been done for $k_F$ and $3k_F$ with the CFT technique [7-9], by obtaining MD and critical exponents at $5k_F$ and $7k_F$. In this study, we used the methods of CFT to establish power-law dependence of the MD and obtained critical exponents at these new Fermi points. The new critical exponents varies monotonically with change in magnetic field, and as $B \to 0$, they are obtained as 25/8 and 49/8 at $5k_F$ and $7k_F$ respectively. However, singularities of MD at $5k_F$ and $7k_F$ Fermi points, appears weaker and gradually degenerating into a smooth curve.

This paper is outlined as follows. Section 1, illustrates the motivation to this study. The mathematical theory is reviewed in section 2. While in section 3, we present analytical calculations of the asymptotic correlation function, MD and critical exponents. Discussion of results and conclusion are shown in section 4 and this is immediately followed by list of references.

2.0 One-dimensional Hubbard Model and Conformal Field Theory approach for Correlation Functions

The Hamiltonian [10] of the HM is given by the expression

$$H = -\sum_{\sigma} (c_{j+\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{j+\sigma}^\dagger) + u \sum_{j} n_{j,\uparrow} n_{j,\downarrow} - \mu \sum_{j} (n_{j,\uparrow} + n_{j,\downarrow}) - \frac{H}{2} \sum_{\sigma} (n_{j,\uparrow} - n_{j,\downarrow})$$

(2.1)

Where $c_{j,\sigma}^\dagger$ is the creation (annihilation) operator with electron spin $\sigma$ at site $j$ and the number operator is $n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$. $u$ is the on-site Coulomb repulsion, $\mu$ is the chemical potential and $H$ is the external magnetic field. The hopping integral $t = 1$. Lieb and Wu (1968) obtained the Bethe-Ansatz solution to Eqn. (2.1) as

$$N k_F = 2\pi I_0 + \frac{N}{N+1} \sum_{j=1}^{N} 2 \tan^{-1} \left( \frac{\sin k_F - \lambda_j}{u} \right)$$

(2.2)

$$\sum_{j=1}^{N} 2 \tan^{-1} \left( \frac{\lambda_j - \sin k_F}{u} \right) = 2\pi J_u + \frac{N}{N+1} \sum_{j=1}^{N} 2 \tan^{-1} \left( \frac{\lambda_j - \lambda_u}{u} \right)$$

(2.3)

The quantum numbers $I_0$ and $J_u$ are integers or half-odd integer depending on the particles of the number of down and up spins, respectively. The state corresponding to the Bethe-Ansatz solution Eqns. (2.2) and (2.3) has energy and momentum given by

$$E_u = \left( I_0 + \Delta^u \right) + O(N)$$

(2.4)

$$P = \left( 2\pi - 2k_F + k_{\downarrow} \right) D_\uparrow + \left( 2\pi - 2k_F \right) D_\downarrow$$

(2.5)

Where the conformal dimensions $\Delta^u$ for the holon (spinon) excitations are given by

$$2\Delta^u = \left( Z_\sigma D_\sigma + Z_\alpha D_\alpha \pm \frac{Z_\Delta N - Z_\Delta N}{2 \det Z} \right)^2 + N^\alpha$$

(2.6)
\[ 2\Delta^{\pm}_n(\Delta N, D) = \left( Z^{c}_{e} D^{e}_{e} + Z^{s}_{s} D^{s}_{s} \pm \frac{Z^{c}_{e} \Delta N^{e}_{e} - Z^{s}_{s} \Delta N^{s}_{s}}{2 \det Z} \right)^2 + 2N^{\pm}_{n} \]  

(2.7)

The positive integers \( N^{\pm}_{n} \), for holon and spinon describes particle-hole excitations, with \( N^{n}_{e} (N^{n}_{s}) \) being the number of occupancies that a particle at the right (left) Fermi level jumps to, \( \Delta N^{n}_{e} (\Delta N^{n}_{s}) \) represents the change in the number of electrons (down-spin) with respect to the ground state, \( D^{e}_{e} \) represents the number of particles which transfer from one Fermi level of the holon to the other and \( D^{s}_{s} \) represents the number of particles which transfer from one Fermi level of the spinon to the other, and both \( D^{e}_{e} \) and \( D^{s}_{s} \) are either integer or half-odd integer values. Finally, \( Z \) is the dressed charge \( 2 \times 2 \) matrix describing anomalous behaviour of critical exponents. The \( 2 \times 2 \) matrix elements are given by

\[ Z^{c}_{c} (k) = 1 + \int_{-\infty}^{\infty} d\lambda a_{c}(k-\lambda)\xi_{c}(\lambda) \]  

(2.8)

\[ Z^{s}_{s}(\lambda) = \int_{-\infty}^{\infty} dk a_{s}(\lambda-k)Z^{c}_{c}(k) - \int_{-\infty}^{\infty} d\mu a_{c}(\lambda-\mu)Z^{s}_{s}(\mu) \]  

(2.9)

\[ Z^{c}_{c}(k) = \int_{-\infty}^{\infty} d\lambda a_{c}(k-\lambda)Z^{c}_{c}(\lambda) \]  

(2.10)

\[ Z^{s}_{s}(\lambda) = 1 + \int_{-\infty}^{\infty} dk a_{s}(\lambda-k)Z^{c}_{c}(k) - \int_{-\infty}^{\infty} d\mu a_{c}(\lambda-\lambda')Z^{s}_{s}(\mu) \]  

(2.11)

Where the kernel is defined as

\[ a_{c}(x) = \frac{2}{\pi} \frac{n u}{(n u)^2 + x^2} \]  

(2.12)

The values of \( \lambda_{0} \) and \( k_{0} \) are usually fixed by

\[ n_{c} = \int_{-\infty}^{\infty} \rho_{c}(k)dk = \int_{-\infty}^{\infty} \frac{Z^{c}_{c}(k)}{2\pi} dk \]  

(2.13)

\[ n_{s} = \int_{-\infty}^{\infty} \rho_{s}(\lambda)d\lambda = \int_{-\infty}^{\infty} \frac{Z^{s}_{s}(\lambda)}{2\pi} d\lambda = \int_{-\infty}^{\infty} Z^{c}_{c}(k) \]  

(2.14)

For small magnetic field Eqns.(2.8) – (2.11) has been solved by Wiener-Hopf technique [8, 11] for terms up to order \( 1/u \) in the strong coupling limit, and obtained the elements to be [see Eqns. (17) to (79) of Ref. 12]

\[ Z^{c}_{c}(k_{0}) = 1 \]  

(2.15)

\[ Z^{s}_{s}(\lambda_{0}) = 0 \]  

(2.16)

\[ Z^{c}_{c}(k_{0}) = \frac{1}{2} - \frac{2}{\pi^{2}} \frac{H}{H_{c}} \]  

(2.17)

\[ Z^{s}_{s}(\lambda_{0}) = \sqrt{2} \left( \frac{1}{2} + \frac{1}{8\ln(H_{c}/H)} \right) \]  

(2.18)

Therefore, the magnetic field dependence of the conformal dimensions Eqns. (2.6) and (2.7) are given by

\[ \Delta^{\pm}_n(\Delta N, D) = \left( (D^{e}_{e} + \frac{\pm D^{s}_{s}}{2}) \pm \frac{\pm \Delta N^{e}_{e}}{2 \det Z} \right)^2 + 2N^{\pm}_{n} \]  

(2.19)
\[ 2\Delta_i^+ = \frac{1}{2} \left( D_i \pm \left( \Delta N_i - \frac{1}{2} \Delta N_s \right) \right)^2 + \frac{2B}{\pi^2 B_i} \left( \Delta N_i \left( D_i \pm \Delta N_s \right) - \frac{1}{2} \left( \Delta N_s \right)^2 \right) + \frac{1}{4\ln(B_c/B)} \left( D_i - \left( \Delta N_i \mp \frac{1}{2} \Delta N_s \right) \right) + 2N_i^+ \]  

(2.20)

Where \( B \) is the external magnetic field, \( B_c \) is the critical field and \( B_s \) is the magnetic field at zero temperature and these are related by

\[ B_s = \frac{\pi^2}{2e} B_c, \]

\[ B_i = 4\pi^2 n_i^0 \left( 1 - \frac{\pi^2 n_i^0}{4u^2} \right); u >> 1 \]

(2.21)

with \( u \) as the strong coupling. However, the Hubbard model is critical at zero temperature [7 - 9] and remarkable progress in the description of critical phenomena has been made by application of the concept of CFT [7, 13]. In the language of conformal field theory, the two point correlation function [7, 10] is given by

\[ G(t,x) \approx \sum_{i,\delta} a_i \exp(-2iDk_{\delta},x) \exp(-2i(D_i + D_s)k_{\delta},x) \]

(2.22)

\[ \frac{1}{(x-ivt)^{i\Delta} (x+ivt)^{i\Delta}} \]

Where \( k_{\delta} \) is the Fermi point with spin \( \sigma \), \( v_i \) is the velocity for holon(spinon) excitations and \( \Delta_{i+}^{i-} \) is right(left) conformal dimension for \( c = \text{holon} \) and \( s = \text{spinon} \) excitations.

### 3.0 Long-Distance Asymptotics for Correlation Functions

Now we use the predictions of conformal field theory outlined in section 2, to obtain the long-distance asymptotic expression. In particular, we want to calculate the electron field correlation function with spin up

\[ G^u_{i+}(t,x) \approx \sum_{i,\delta} a_i \exp(-2iDk_{\delta},x) \exp(-2i(D_i + D_s)k_{\delta},x) \]

(3.1)

Here, both \( D_i \) and \( D_s \) take half-odd integer, \( \Delta N_i = 1, \Delta N_s = 0 \) and \( N_i^0 = 0 \). Our calculations are done for the quantum numbers \( (N_i^+, \Delta N_i, \Delta N_s, D_i, D_s) = (0, 1, 0, -1/2, 1/2), (0, 1, 0, -1/2, -1/2), (0, 1, 0, 3/2, -1/2) \) and \( (0, 1, 0, -3/2, -1/2) \). Therefore, the corresponding conformal dimensions for \( 0, 1, 0, -1/2, 1/2 \) are obtained as

\[ 2\Delta_i^+ = \frac{1}{16} \frac{B}{\pi^2 B_i}, \quad 2\Delta_s^+ = \frac{9}{16} + \frac{3B}{\pi^2 B_i} \]

(3.2)

\[ 2\Delta_i^- = 0, \quad 2\Delta_s^- = \frac{1}{2} \]

(3.3)

Eqs. (3.2) and (3.3) are contributions from the holon and spinon excitations respectively. For \( 0, 1, 0, -1/2, -1/2 \), we obtain conformal dimensions corresponding to the holon and spinon excitations as

\[ 2\Delta_i^+ = \frac{1}{16} \frac{B}{2\pi^2 B_i}, \quad 2\Delta_s^+ = \frac{25}{16} - \frac{5B}{2\pi^2 B_i} \]

(3.4)

\[ 2\Delta_i^- = \frac{1}{2} - \frac{2B}{\pi^2 B_i}, \quad 2\Delta_s^- = -\frac{2B}{\pi^2 B_i} \]

(3.5)

For quantum number \( 0, 1, 0, 3/2, -1/2 \), we obtain conformal dimensions corresponding to the holon and spinon excitations as

\[ 2\Delta_i^+ = \frac{49}{16} + \frac{7B}{2\pi^2 B_i}, \quad 2\Delta_s^+ = \frac{9}{16} + \frac{3B}{2\pi^2 B_i} \]

(3.6)
Finally, for the quantum number \((0, 1, 0, -3/2, -1/2)\), contributions from holon and spinon excitations are obtained as

\[
2\Delta_1^v = \frac{25}{16} \frac{5B}{2\pi^2 B}, \quad 2\Delta_1^- = \frac{81}{16} \frac{9B}{2\pi^2 B}, \quad 2\Delta_2^v = \frac{1}{2} \frac{2B}{\pi^2 B}, \quad 2\Delta_2^- = -\frac{2B}{\pi^2 B} \tag{3.8}
\]

Using the results of conformal dimensions Eqns. (3.2) – (3.9) on Eqn. (3.1), we obtain the long-distance asymptotic expression for electron field correlation function with spin up as

\[
G^v_{\psi\psi}(t,x) \approx \frac{a_1 \cos(k_{r,z} x)}{[x + iv t]^{\theta_1}} + \frac{a_2 \cos((k_{r,z} + 2k_{r,x}) x)}{[x + iv t]^{\theta_2}} + \frac{a_3 \cos((3k_{r,z} + 3k_{r,x}) x)}{[x + iv t]^{\theta_3}} + \frac{a_4 \cos((3k_{r,z} + 4k_{r,x}) x)}{[x + iv t]^{\theta_4}} \tag{3.10}
\]

Note that the Fermi point \(3k_{r,z}\) manifests as \(k_{r,z} + 2k_{r,x}\), \(5k_{r,z}\) as \(3k_{r,z} + 2k_{r,x}\) and \(7k_{r,z}\) as \(3k_{r,z} + 4k_{r,x}\) respectively.

Where the exponents are given by

\[
\theta_1 = 2\Delta_1^v + 2\Delta_1^- = \frac{5}{8} + \frac{2B}{\pi^2 B}, \quad \theta_2 = 2\Delta_2^v + 2\Delta_2^- = \frac{1}{2} \tag{3.11}
\]

\[
\theta_3 = \frac{13}{8} - \frac{3B}{\pi^2 B}, \quad \theta_4 = \frac{1}{2} - \frac{4B}{\pi^2 B} \tag{3.12}
\]

\[
\theta_5 = \frac{29}{8} + \frac{5B}{\pi^2 B}, \quad \theta_6 = \frac{1}{2} - \frac{4B}{\pi^2 B} \tag{3.13}
\]

\[
\theta_7 = \frac{53}{8} - \frac{7B}{\pi^2 B}, \quad \theta_8 = \frac{1}{2} - \frac{4B}{\pi^2 B} \tag{3.14}
\]

### 3.1 Momentum Distribution Function

The long-distance asymptotic expression Eqn. (3.10) has singularities near the Fermi points \(k_{r,z}\), \(3k_{r,z}\), \(5k_{r,z}\) and \(7k_{r,z}\) respectively. Therefore, the momentum distribution at \(k_{r,z}\) is given by Eqn. (3.15) with critical exponent \(\theta_1\)

\[
\tilde{G}^v(k \approx k_{r,z}) \approx \text{sgn}(k - k_{r,z}) |k - k_{r,z}|^{\theta_1} \tag{3.15}
\]

\[
\theta_1 = \theta_{1v} + \theta_{1s} = \frac{1}{8} + \frac{2B}{\pi^2 B} \tag{3.16}
\]

We determine the exponent by plotting in Fig. 1(a) \(\theta_1\) versus magnetic field \(B/B_c\) and get \(\theta_1 \approx 1/8\) as \(B \to 0\). This value has been obtained earlier [1 - 4, 9, 14]. The MD, \(\tilde{G}^v(k)\) is plotted in Fig. 2(a), and its singularity at \(k \approx k_{r,z}\) is obvious.
The next singularity occurs at $3k_f$, with momentum distribution and critical exponent given Eqns. (3.17) and (3.18) respectively.

$$\tilde{G}^+(k \approx k_{r,\uparrow} + 2k_{r,\downarrow}) \approx \text{sgn}(k - k_{r,\uparrow} - 2k_{r,\downarrow})|k - k_{r,\uparrow} - 2k_{r,\downarrow}|^\theta$$  \hspace{1cm} (3.17)

$$\theta = \theta_2 + \theta_2 - 1 + \frac{9}{8} \frac{7B}{\pi^2B}$$ \hspace{1cm} (3.18)

We plot in Fig. 1(b), the exponent $\theta_2$ versus magnetic field $B/B_\varphi$ and get $\theta_2 \mid 9/8$ as $B \to 0$. The singularity at $k \approx 3k_f$ is shown in Fig. 2(b). The momentum distribution, $\tilde{G}^+(k)$ decreases continuously to a point $k = 0.75\pi$, where discontinuity occur. Thereafter, $\tilde{G}^+(k)$ begins to increase again. Near $5k_f$ and $7k_f$, the momentum distribution and critical exponents are obtained as

$$\tilde{G}^+(k \approx 3k_{r,\uparrow} + 2k_{r,\downarrow}) \approx \text{sgn}(k - 3k_{r,\uparrow} - 2k_{r,\downarrow})|k - 3k_{r,\uparrow} - 2k_{r,\downarrow}|^\theta$$ \hspace{1cm} (3.19)
\[
\theta_{s} = \theta_{s} + \theta_{s} - 1 = \frac{25}{8} + \frac{B}{\pi^2 B}.
\]

\[
\tilde{G}^+(k \approx 3k_x + 4k_y) = \text{sgn}(k - 3k_x - 4k_y) \left| k - 3k_x - 4k_y \right|^\theta
\]

\[
\theta_{s} = \theta_{s} + \theta_{s} - 1 = \frac{49}{8} - \frac{11B}{\pi^2 B}
\]

We get \( \theta_s \approx 25/8 \) and \( \theta_s \approx 49/8 \) by plotting critical exponent \( \theta_{s} \) and \( \theta_{s} \) versus magnetic field \( B/B_c \) as shown in Fig. 3. Weaker singularities at \( 5k_x \) and \( 7k_x \) are noticed in the plots for \( \tilde{G}^+(k) \) in Fig. 4. This may be due to increase in number of particles which transfer from one Fermi level of the holon to the other.

Fig. 3. Critical exponents \( \theta_{s} \) and \( \theta_{s} \) for the momentum distribution at (a) \( 5k_x \) and (b) \( 7k_x \) versus magnetic field \( B/B_c \).

Fig. 4. Momentum distribution functions \( \tilde{G}^+ \) of (a) \( 5k_x \) and (b) \( 7k_x \) singularities in the electron field correlation function in the 1D Hubbard model.
4.0 Discussion

It is clear from the critical exponent equations given by (3.16), (3.18), (3.20) and (3.22), that exponents of the momentum distribution which characterizes the Tomonaga-Luttinger liquid in contrast to the usual Fermi liquid theory depends on the magnetic field. When \( B \to 0 \), the critical exponents are obtained as 1/8, 9/8, 25/8 and 49/8 at various Fermi points. Power-law singularity occurs at the Fermi points \( k_r \), \( 3k_r \), \( 5k_r \) and \( 7k_r \), respectively. This singularity behaviour appears around \( k = 0.25\pi \) and \( k = 0.75\pi \) for \( k_r \) and \( 3k_r \), as shown in Fig. 2. The calculated exponents for the MD singularities at \( k_r \) and \( 3k_r \) agree with the results from numerical study. The calculated exponent for the MD at \( 5k_r \) is significantly 25/8 and indicates there is weak singularity near this point. This result disagrees with the numerical prediction of 1. We obtained an exponent of 49/8 at \( 7k_r \). However, singularities at \( 5k_r \) and \( 7k_r \) appears weaker and gradually degenerating into a smooth curve. This property at \( 5k_r \) and \( 7k_r \) may lead to better understanding of Tomonaga-Luttinger liquid. This can be examined further to explore the physics involved.

References


