

Finite size effects for the gap in the excitation spectrum of the one-dimensional Hubbard model

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We study finite size effects for the gap of the quasiparticle excitation spectrum in the weakly interacting regime one-dimensional Hubbard model with on-site attraction. Two type of corrections to the result of the thermodynamic limit are obtained. Aside from a power law (conformal) correction due to gapless excitations which behaves as $1/N_a$, where N_a is the number of lattice sites, we obtain corrections related to the existence of gapped excitations. First of all, there is an exponential correction which in the weakly interacting regime ($|U| \ll t$) behaves as $\sim \exp(-N_a \Delta_\infty / 4t)$ in the extreme limit of $N_a \Delta_\infty / t \gg 1$, where t is the hopping amplitude, U is the on-site energy, and Δ_∞ is the gap in the thermodynamic limit. Second, in a finite size system a spin-flip producing unpaired fermions leads to the appearance of solitons with non-zero momenta, which provides an extra (non-exponential) contribution δ . For moderate but still large values of $N_a \Delta_\infty / t$, these corrections significantly increase and may become comparable with the $1/N_a$ conformal correction. Moreover, in the case of weak interactions where $\Delta_\infty \ll t$, the exponential correction exceeds higher order power law corrections in a wide range of parameters, namely for $N_a \lesssim (8t/\Delta_\infty) \ln(4t/|U|)$, and so does δ even in a wider range of N_a . For sufficiently small number of particles, which can be of the order of thousands in the weakly interacting regime, the gap is fully dominated by finite size effects.

I. INTRODUCTION

The one-dimensional (1D) Hubbard model with only on-site interaction is exactly solvable by the Bethe Ansatz, and the properties of this model have been widely studied [1]. Low lying excitations of the Hubbard model with attraction are gapless charge excitations and gapped spin excitations, whereas for the repulsive model the gap exists only at half filling in the charge sector.

Finite size corrections to the ground state energy E_0 , due to the gapless part of the spectrum, follow from conformal field theory [2, 3, 4, 5] and have the form: $E_0 - \epsilon_0 L = -\pi v \hbar / 6L$, where $L = N_a a$ is the size of the system, N_a is the number of lattice sites, a is the lattice constant, ϵ_0 is the energy per unit length in the thermodynamic limit, and v is the velocity of gapless excitations. Finite size corrections to the energies of low-lying gapless excitations are also proportional to v/N_a , and the proportionality coefficient depends on the scaling dimensions of the primary fields. However, finite size corrections originating from the gapped sector remained unknown for the Hubbard model. Finite size effects are expected to be important for sufficiently small systems, such as cold atoms in a 1D optical lattice, where the number of particles and lattice sites ranges from several tens to several hundreds [6, 7].

In this paper we solve the Bethe Ansatz equations for a finite number of particles and calculate finite size corrections to the gap for the attractive Hubbard model. As expected, there are power law $1/N_a$ corrections due to gapless excitations, and we also find contributions related to the existence of gapped excitations. First of all, there is an exponential correction which in the weakly interacting regime ($|U| \ll t$) behaves as $\sim \exp(-N_a \Delta_\infty / 4t)$ in the extreme limit of $N_a \Delta_\infty / t \gg 1$, where t is the hopping amplitude, U is the on-site interaction, and Δ_∞ is the gap in the thermodynamic limit. Second, in a finite size system a spin-flip producing unpaired fermions leads to the appearance of solitons with non-zero momenta, which provides an extra (non-exponential) contribution. For moderate but still large values of $N_a \Delta_\infty / t$, these corrections may become comparable with the $1/N_a$ conformal correction. Moreover, in the case of weak interactions where $\Delta_\infty \ll t$, the exponential correction exceeds higher order power law corrections in a wide range of parameters, namely for $N_a \lesssim (8t/\Delta_\infty) \ln(4t/|U|)$, and so does δ even in a wider range of N_a . We find that the value of the gap increases with decreasing the system size and show how the gap becomes dominated by finite size effects in sufficiently small systems.

The paper is organized as follows. In section II we introduce the Hubbard model together with related Bethe Ansatz equations, and discuss the thermodynamic limit. In section III we present a general approach for finding finite size corrections to the ground state energy and to the gap and discuss the structure of the gap. Section IV contains our results for corrections due to the gapped sector at half filling, and section V the results for power law corrections. In Section VI we discuss our numerical and analytical results, and in Section VII present for completeness a perturbative

approach for solving the Bethe Ansatz equations in the limiting case of $L \ll at/U$. In Section VIII we conclude.

II. GENERAL EQUATIONS, THERMODYNAMIC LIMIT

The Hubbard model for a system of interacting spin-1/2 fermions on a lattice is described by the Hamiltonian

$$H = -t \sum_{\sigma=\uparrow,\downarrow; j=1}^{N_a} (c_{j,\sigma}^\dagger c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger c_{j,\sigma}) + U \sum_{j=1}^{N_a} n_{j,\uparrow} n_{j,\downarrow}, \quad (1)$$

where the subscript j labels the lattice sites. The index σ labels the spin projection, $c_{j,\sigma}^\dagger$ and $c_{j,\sigma}$ are the creation and annihilation fermion operators, and $n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$ are the particle number operators. Below we express all quantities having the dimension of energy in units of t , and quantities having the dimension of length in units of the lattice constant a .

Lieb and Wu have solved the Fermi-Hubbard model by means of the Bethe Ansatz [8]. The corresponding eigenvalue equations read

$$\sum_{j=1}^N 2 \arctan \left(\frac{\lambda_\alpha - \sin k_j}{u} \right) = 2\pi J_\alpha + \sum_{\beta=1}^M 2 \arctan \left(\frac{\lambda_\alpha - \lambda_\beta}{2u} \right), \quad \alpha = 1, \dots, M, \quad (2)$$

$$N_a k_j = 2\pi I_j - \sum_{\beta=1}^M 2 \arctan \left(\frac{\sin k_j - \lambda_\beta}{u} \right), \quad j = 1, \dots, N, \quad (3)$$

where $u = |U|/4t$, M is the number of spin-down fermions, and N is the total number of particles. The energy of a given state is expressed through the charge momenta k_j :

$$E_N = -2 \sum_{j=1}^N \cos k_j, \quad (4)$$

and it depends on the spin rapidities λ_α only implicitly through the coupled equations (2) and (3). For the ground state the quantum numbers I_j and J_α are integers or half-odd integers depending on the parities of N and M :

$$J_\alpha = \frac{N + M + 1}{2} (\text{mod } 1), \quad I_j = \frac{M}{2} (\text{mod } 1). \quad (5)$$

For the Hubbard model with attraction ($U < 0$), there is a gap in the spectrum of spin excitations. Considering a finite number of particles we define the gap Δ as:

$$2\Delta = E_{N+2}(N_\uparrow + 2, N_\downarrow, U) + E_{N-2}(N_\uparrow - 2, N_\downarrow, U) - 2E_N(N_\uparrow, N_\downarrow, U), \quad (6)$$

where $E_N(N_\uparrow, N_\downarrow; U)$ is the ground state energy for a system with N_\uparrow spin-up and $N_\downarrow = N - N_\uparrow$ spin-down fermions in a lattice with N_a lattice sites, at the interaction strength U . This definition is convenient as it does not change the parity of the quantum numbers I_j and J_α . Without loss of generality, we may put $N_\downarrow \leq N_\uparrow$.

In the thermodynamic limit, where $N \rightarrow \infty$ and $N_a \rightarrow \infty$ while keeping constant densities $n = N/L$ and $n_\downarrow = N_\downarrow/L$, Eq. (6) leads to the same result as the definition $\Delta = E_{N_a}(N_\uparrow + 1, N_\downarrow; U) - 2E_{N_a}(N_\uparrow, N_\downarrow; U) + E_{N_a}(N_\uparrow - 1, N_\downarrow; U)$ introduced in Refs. [8, 14].

In the thermodynamic limit the density of momenta k and the density of rapidities λ are defined as $\rho(k) = L^{-1} \partial I / \partial k$ and $\sigma(\lambda) = L^{-1} \partial J / \partial \lambda$, respectively. Then, the Bethe Ansatz equations for the ground state of the repulsive model become:

$$\rho_\infty(k) = \frac{1}{2\pi} + \frac{\cos k}{\pi} \int_{-B}^B \frac{u}{u^2 + (\lambda - \sin k)^2} \sigma_\infty(\lambda) d\lambda, \quad (7)$$

$$\sigma_\infty(\lambda) + \frac{1}{\pi} \int_{-B}^B \frac{2u}{4u^2 + (\lambda - \lambda')^2} \sigma_\infty(\lambda') d\lambda' = \frac{1}{\pi} \int_{-Q}^Q \frac{u}{u^2 + (\lambda - \sin k)^2} \rho_\infty(k) dk, \quad (8)$$

where the constants B and Q are given by

$$\frac{N}{N_a} = n = \int_{-Q}^Q \rho_\infty(k) dk, \quad \frac{N_\downarrow}{N_a} = n_\downarrow = \int_{-B}^B \sigma_\infty(\lambda) d\lambda, \quad (9)$$

and the ground state energy follows from the relation:

$$E_\infty = -2N_a \int_{-Q}^Q \rho_\infty(k) \cos k \, dk. \quad (10)$$

The value of the spin gap for an arbitrary filling factor has been calculated in the thermodynamic limit in Refs. [14, 15]. In the case of weak attraction the result is

$$\Delta_\infty = \frac{16 \sin^{3/2}(\pi n/2) \sqrt{u}}{\pi} \exp\left(-\frac{\pi \sin(\pi n/2)}{2u}\right), \quad (11)$$

and the validity of Eq. (11) requires large values of the exponent.

The particle-hole symmetry and the symmetry with respect to interchanging spin-up and spin-down fermions allow one to establish relations between ground state energies of the repulsive and attractive Hubbard models [8]:

$$\begin{aligned} E(N_\uparrow, N_\downarrow; U) &= -(N_a - N_\uparrow - N_\downarrow)U + E(N_a - N_\uparrow, N_a - N_\downarrow; U) \\ &= N_\uparrow U + E(N_\uparrow, N_a - N_\downarrow; -U) = N_\downarrow U + E(N_a - N_\uparrow, N_\downarrow; -U). \end{aligned} \quad (12)$$

Using Eqs. (6) and (12) we can express the spin gap for the attractive Hubbard model through the energies of the repulsive model:

$$2\Delta = 2|U| + E_{N_a-2}(M-2, N_a-M, |U|) + E_{N_a-2}(N_a-M-2, M, |U|) - 2E_{N_a}(M, N_a-M, |U|). \quad (13)$$

For the half-filled case ($N = 2M = N_a$), with $N_\uparrow = N_\downarrow = M$, Eq. (13) takes the form:

$$\Delta = |U| + E_{N_a-2}(N_a/2, N_a/2 - 2, |U|) - E_{N_a}(N_a/2, N_a/2, |U|). \quad (14)$$

Below we calculate the gap for the attractive Hubbard model. For this purpose we first perform calculations of ground state energies for the repulsive Hubbard model, where the momenta k_j are real numbers, and then obtain Δ for the attractive model by using Eq. (13) (Eq. (14) for the half filled case). This allows us to find exponential finite size corrections, which is not possible in direct calculations for the case of attraction where k_j are complex and can be found only with an exponential accuracy.

III. FINITE SIZE CORRECTIONS. GENERAL APPROACH

Thus, in order to calculate finite size corrections to the gap we have to obtain the three energies of a finite size system, entering the right hand side of Eq. (13). We will follow the scheme proposed by de Vega and Woynarovich [10], which introduces a formalism allowing us to use the Bethe Ansatz in order to calculate finite size corrections to the energy of the ground state. The scheme consists of writing the Bethe Ansatz equations (2) and (3) in the form:

$$Z^s(\lambda) = \frac{1}{N_a} \sum_j^N \frac{1}{\pi} \arctan \frac{\lambda - \sin k_j}{u} - \frac{1}{N_a} \sum_\beta^M \frac{1}{\pi} \arctan \frac{\lambda - \lambda_\beta}{2u}, \quad Z^s(\lambda_\alpha) = \frac{J_\alpha}{N_a}, \quad (15)$$

$$Z^c(k) = \frac{k}{2\pi} + \frac{1}{N_a} \sum_\alpha^M \frac{1}{\pi} \arctan \frac{\sin k - \lambda_\alpha}{u}, \quad Z^c(k_j) = \frac{I_j}{N_a}. \quad (16)$$

We then define the densities of momenta k and rapidities λ for a finite size system as

$$\sigma_N(\lambda) \equiv \frac{dZ^s}{d\lambda} = \frac{1}{2\pi N_a} \sum_{j=1}^N K_1(\lambda - \sin k_j) - \frac{1}{2\pi N_a} \sum_{\beta=1}^M K_2(\lambda - \lambda_\beta), \quad (17)$$

$$\rho_N(k) \equiv \frac{dZ^c}{dk} = \frac{1}{2\pi} + \frac{1}{N_a} \frac{\cos k}{2\pi} \sum_{\alpha=1}^M K_1(\sin k - \lambda_\alpha), \quad (18)$$

where $K_1(x) = 2u/(u^2 + x^2)$, and $K_2 = 4u/(4u^2 + x^2)$. The densities satisfy the relations:

$$\int_{\Lambda_-}^{\Lambda_+} \sigma_N(\lambda) d\lambda = \frac{M}{N_a}, \quad \int_{Q_-}^{Q_+} \rho_N(k) dk = \frac{N}{N_a}, \quad (19)$$

where Q_{\pm}, Λ_{\pm} are determined from the equations

$$Z^c(Q_+) = \frac{I_+}{N_a} = \frac{I_{max} + 1/2}{N_a}; \quad Z^s(\Lambda_+) = \frac{J_+}{N_a} = \frac{J_{max} + 1/2}{N_a}. \quad (20)$$

We first perform calculations for the half-filled case. According to Eq. (14) we have to calculate $E_{N_a}(N_a/2, N_a/2; |U|)$ and $E_{N_a}(N_a/2, N_a/2 - 2; |U|)$. In the former case we have $N = N_a$ and $N_{\uparrow} = N_{\downarrow} = N_a/2 = M$, and the quantum numbers for the ground state are

$$\begin{aligned} J_{\alpha} &= \left\{ -\frac{M-1}{2}, \dots, -1, 0, 1, \dots, \frac{M-1}{2} \right\}, \\ I_j &= \left\{ -\frac{N-1}{2}, \dots, -\frac{1}{2}, \frac{1}{2}, \dots, \frac{N-1}{2} \right\}. \end{aligned} \quad (21)$$

With $N = N_a$ and $M = N_a/2$, from Eq. (21) we have

$$J_{max} = \frac{N_a/2 - 1}{2}; \quad I_{max} = \frac{N_a - 1}{2}. \quad (22)$$

Then, from Eq. (20) we obtain

$$\begin{aligned} J_+ &= \frac{N_a}{4}, \quad Z_s(\Lambda_+) = \frac{1}{4}, \\ I_+ &= \frac{N_a}{2}, \quad Z_c(Q_+) = \frac{1}{2}, \end{aligned} \quad (23)$$

and Eqs. (15) and (16) lead to

$$\Lambda_+ = \infty; \quad Q_+ = \pi. \quad (24)$$

When calculating the energy $E_{N_a}(N_a/2, N_a/2 - 2; |U|)$ we have $N = N_a - 2$, $N_{\uparrow} = N_a/2$, and $N_{\downarrow} = N_a/2 - 2$. It is convenient to introduce two additional particles with momenta $k_h = \{k_1, k_{N_a}\}$ and spin rapidities $\lambda_h = \{\lambda_1, \lambda_{N_a/2}\}$ in order to satisfy the conditions $Q_{\pm} = \pm\pi$ and $\Lambda_{\pm} = \pm\infty$. The discrete Bethe Ansatz equations in this case read

$$\begin{aligned} &\sum_{j=1}^{N_a} 2 \arctan \left(\frac{\lambda_{\alpha} - \sin k_j}{u} \right) = 2\pi J_{\alpha} + \sum_{\beta=1}^{N_a/2} 2 \arctan \left(\frac{\lambda_{\alpha} - \lambda_{\beta}}{2u} \right) \\ &+ \sum_{k_h} 2 \arctan \left(\frac{\lambda_{\alpha} - \sin k_h}{u} \right) - \sum_{\lambda_h} 2 \arctan \left(\frac{\lambda_{\alpha} - \lambda_h}{2u} \right), \quad \alpha = 1, \dots, N_a/2, \end{aligned} \quad (25)$$

$$N_a k_j = 2\pi I_j - \sum_{\beta=1}^{N_a/2} 2 \arctan \left(\frac{\sin k_j - \lambda_{\beta}}{u} \right) + \sum_{\lambda_h} 2 \arctan \left(\frac{\sin k_j - \lambda_h}{u} \right), \quad j = 1, \dots, N_a. \quad (26)$$

Note that we added only 4 additional equations for defining the numbers k_h, λ_h . Other equations are exactly the Bethe Ansatz equations for $N_a - 2$ particles. The sets J_{α}, I_j are the same as for the ground state of N_a particles (21).

For the case $N = N_a$ we rewrite equations (17) and (18) in the form of integral equations for the densities $\sigma_{N_a}(\lambda), \rho_{N_a}(k)$:

$$\begin{aligned} \sigma_{N_a}(\lambda) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} K_1(\lambda - \sin k) \rho_{N_a}(k) dk - \frac{1}{2\pi} \int_{-\infty}^{\infty} K_2(\lambda - \mu) \sigma_{N_a}(\mu) d\mu \\ &+ \frac{1}{2\pi} \int_{-\pi}^{\pi} K_1(\lambda - \sin k) X_{N_a}^c(k) dk - \frac{1}{2\pi} \int_{-\infty}^{\infty} K_2(\lambda - \mu) X_{N_a}^s(\mu) d\mu, \end{aligned} \quad (27)$$

$$\begin{aligned} \rho_{N_a}(k) &= \frac{1}{2\pi} + \frac{1}{2\pi} \int_{-\infty}^{\infty} K_1(\sin k - \lambda) \cos k \sigma_{N_a}(\lambda) d\lambda \\ &+ \frac{1}{2\pi} \int_{-\infty}^{\infty} \cos k K_1(\sin k - \lambda) X_{N_a}^s(\lambda) d\lambda, \end{aligned} \quad (28)$$

with the quantities $X_{N_a}^s$ and $X_{N_a}^c$ defined as

$$X_{N_a}^c(k) = \frac{1}{N_a} \left[\sum_{j=1}^{N_a} \delta(k - k_j) \right] - \rho_{N_a}(k), \quad (29)$$

$$X_{N_a}^s(\lambda) = \frac{1}{N_a} \left[\sum_{\alpha=1}^{N_a/2} \delta(\lambda - \lambda_\alpha) \right] - \sigma_{N_a}(\lambda). \quad (30)$$

For $N = N_a - 2$ we do the same and obtain

$$\begin{aligned} \sigma_{N_a-2}(\lambda) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} K_1(\lambda - \sin k) \rho_{N_a-2}(k) dk - \frac{1}{2\pi} \int_{-\infty}^{\infty} K_2(\lambda - \mu) \sigma_{N_a-2}(\mu) d\mu \\ &+ \frac{1}{2\pi} \int_{-\pi}^{\pi} K_1(\lambda - \sin k) X_{N_a-2}^c(k) dk - \frac{1}{2\pi} \int_{-\infty}^{\infty} K_2(\lambda - \mu) X_{N_a-2}^s(\mu) d\mu \\ &- \frac{1}{2\pi N_a} \sum_{k_h} K_1(\lambda - \sin k_h) + \frac{1}{2\pi N_a} \sum_{\lambda_h} K_2(\lambda - \lambda_h), \end{aligned} \quad (31)$$

$$\begin{aligned} \rho_{N_a-2}(k) &= \frac{1}{2\pi} + \frac{1}{2\pi} \int_{-\infty}^{\infty} K_1(\sin k - \lambda) \sigma_{N_a-2}(\lambda) \cos k d\lambda \\ &+ \frac{1}{2\pi} \int_{-\infty}^{\infty} K_1(\sin k - \lambda) X_{N_a-2}^s(\lambda) \cos k d\lambda - \frac{1}{2\pi N_a} \sum_{\lambda_h} K_1(\sin k - \lambda_h) \cos k. \end{aligned} \quad (32)$$

The functions $X_{N_a-2}^{s,c}$ are given by

$$X_{N_a-2}^s(\lambda) = \frac{1}{N_a} \sum_{\alpha=1}^{N_a/2} \delta(\lambda - \lambda_\alpha) - \sigma_{N_a-2}(\lambda), \quad (33)$$

$$X_{N_a-2}^c(k) = \frac{1}{N_a} \sum_{j=1}^{N_a} \delta(k - k_j) - \rho_{N_a-2}(k), \quad (34)$$

where the summation over k_j , λ_α includes the additional numbers k_h , λ_h .

We first consider the thermodynamic limit where the terms $X^{s,c}$ in Eqs. (27), (28), (31) and (32) vanish. For the half-filled case of $N = N_a$ the solution is known [8]:

$$\rho_{\infty, N_a}(k) = \frac{1}{2\pi} + \frac{\cos k}{2\pi} \int_0^{\infty} \frac{\cos(\omega \sin k) \exp(-\omega u)}{\cosh \omega u} J_0(\omega) d\omega, \quad (35)$$

$$\sigma_{\infty, N_a}(\lambda) = \frac{1}{2\pi} \int_0^{\infty} \frac{\cos \omega \lambda}{\cosh \omega u} J_0(\omega) d\omega. \quad (36)$$

Integrating the density of momenta over dk we obtain

$$Z_{\infty, N_a}^c(k) = \frac{k}{2\pi} + \frac{1}{2\pi} \int_0^{\infty} \frac{\sin(\omega \sin k) \exp(-\omega u)}{\omega \cosh \omega u} J_0(\omega) d\omega. \quad (37)$$

For the case of $N = N_a - 2$ the solution is easily found:

$$\begin{aligned} \sigma_{\infty, N_a-2} &= \sigma_{\infty, N_a} - \frac{1}{2\pi N_a} \sum_{k_h} \frac{\pi}{2u} \frac{1}{\cosh[\pi(\lambda - \sin k_h)/2u]} \\ &+ \frac{1}{2\pi N_a} \sum_{\lambda_h} \int_0^{\infty} \frac{\cos[\omega(\lambda - \lambda_h)]}{\cosh \omega u} \exp(-\omega u) d\omega, \end{aligned} \quad (38)$$

$$\begin{aligned} \rho_{\infty, N_a-2} &= \rho_{\infty, N_a} - \frac{\cos k}{2\pi N_a} \sum_{k_h} \int_0^{\infty} \frac{\cos[\omega(\sin k - \sin k_h)]}{\cosh \omega u} \exp(-\omega u) d\omega \\ &- \frac{\cos k}{2\pi N_a} \sum_{\lambda_h} \frac{\pi}{2u} \frac{1}{\cosh[\pi(\sin k - \lambda_h)/2u]}, \end{aligned} \quad (39)$$

and

$$Z_{\infty, N_a-2}^c(k) = Z_{\infty, N_a}^c(k) - \frac{1}{2\pi N_a} \sum_{k_h} \int_0^\infty \frac{\sin[\omega(\sin k - \sin k_h)] \exp(-\omega u)}{\omega \cosh \omega u} d\omega$$

$$- \frac{1}{2\pi N_a} \sum_{\lambda_h} 2 \arctan \left[\tanh \left(\frac{\pi}{4u} (\sin k - \lambda_h) \right) \right]. \quad (40)$$

For calculating the finite size corrections we should find the differences between the densities $\rho_{N_a}(k)$, $\sigma_{N_a}(\lambda)$, $\sigma_{N_a-2}(\lambda)$, $\rho_{N_a-2}(k)$ and their thermodynamic limit values. Subtracting equations of the thermodynamic limit from Eqs. (27), (28) for the case $N = N_a$ we obtain:

$$\delta\sigma_{N_a}(\lambda) = \sigma_{N_a}(\lambda) - \sigma_{\infty, N_a}(\lambda) = \frac{1}{2\pi} \int_{-\pi}^{\pi} K_1(\lambda - \sin k) \delta\rho_{N_a}(k) dk - \frac{1}{2\pi} \int_{-\infty}^{\infty} K_2(\lambda - \mu) \delta\sigma_{N_a}(\mu) d\mu$$

$$+ \frac{1}{2\pi} \int_{-\pi}^{\pi} K_1(\lambda - \sin k) X_{N_a}^c(k) dk - \frac{1}{2\pi} \int_{-\infty}^{\infty} K_2(\lambda - \mu) X_{N_a}^s(\mu) d\mu, \quad (41)$$

$$\delta\rho_{N_a}(k) = \rho_{N_a}(k) - \rho_{\infty, N_a}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} K_1(\sin k - \lambda) \cos k \delta\sigma_{N_a}(\lambda) d\lambda$$

$$+ \frac{1}{2\pi} \int_{-\infty}^{\infty} \cos k K_1(\sin k - \lambda) X_{N_a}^s(\lambda) d\lambda. \quad (42)$$

Equations (41) and (42) lead to algebraic equations for the Fourier transforms of $\delta\sigma_{N_a}(\lambda)$ and $\delta\rho_{N_a}(k)$, which yields:

$$\delta\sigma_{N_a}(\lambda) = \int_{-\pi}^{\pi} \frac{\pi}{2u \cosh[\pi(\lambda - \sin k)/2u]} X_{N_a}^c(k) \frac{dk}{2\pi}$$

$$- \int_{-\infty}^{\infty} d\mu \int_0^\infty \frac{\cos[\omega(\lambda - \mu)]}{\cosh(\omega u)} \exp(-\omega u) X_{N_a}^s(\mu) \frac{d\omega}{2\pi}. \quad (43)$$

$$\delta\rho_{N_a}(k) = \cos k \int_0^\infty \frac{d\omega}{2\pi} \int_{-\pi}^{\pi} \frac{\exp(-\omega u)}{\cosh(\omega u)} \cos[\omega(\sin k - \sin q)] X_{N_a}^c(q) dq$$

$$+ \frac{\cos k}{2\pi} \int_{-\infty}^{\infty} \frac{\pi}{2u \cosh[\pi(\sin k - \lambda)/2u]} X_{N_a}^s(\lambda) d\lambda. \quad (44)$$

Equations for $\delta\sigma_{N_a-2}(\lambda)$ and $\delta\rho_{N_a-2}(k)$ are obtained in a similar way taking into account that in the thermodynamic limit $k_h = \pm\pi$ and $\lambda_h = \pm\infty$. This gives Eqs. (41), (42) and (43), (44) where N_a is replaced by $N_a - 2$ and $X^{s,c}$ by $\tilde{X}^{s,c}$. The quantity $\tilde{X}_{N_a-2}^s$ is given by Eq.(33) in which the values of λ_h are put equal to $+\infty$ and $-\infty$:

$$\tilde{X}_{N_a-2}^s(\lambda) = \frac{1}{N_a} \sum_{\alpha=1}^{N_a/2-2} \delta(\lambda - \lambda_\alpha) - \sigma_{N_a-2}(\lambda), \quad (45)$$

and $\tilde{X}_{N_a-2}^c$ by Eq. (34) where the values k_h are put equal to $+\pi$ and $-\pi$:

$$\tilde{X}_{N_a-2}^c(k) = \frac{1}{N_a} \left[\sum_{j=1}^{N_a-2} \delta(k - k_j) + \delta(k - \pi) + \delta(k + \pi) \right] - \rho_{N_a-2}(k). \quad (46)$$

The ground state energies (4) for the considered states can be rewritten as

$$\frac{E_{N_a}}{N_a} = -2 \int_{-\pi}^{\pi} \rho_{N_a}(k) \cos k dk - 2 \int_{-\pi}^{\pi} X_{N_a}^c(k) \cos k dk, \quad (47)$$

$$\frac{E_{N_a-2}}{N_a} = -2 \int_{-\pi}^{\pi} \rho_{N_a-2}(k) \cos k dk - 2 \int_{-\pi}^{\pi} X_{N_a-2}^c(k) \cos k dk + \frac{2}{N_a} \sum_{k_h} \cos k_h$$

$$= -2 \int_{-\pi}^{\pi} \rho_{N_a-2}(k) \cos k dk - 2 \int_{-\pi}^{\pi} \tilde{X}_{N_a-2}^c(k) \cos k dk - \frac{4}{N_a}. \quad (48)$$

The finite size corrections to the ground state energy are given by

$$\delta E_N = E_N - E_{\infty, N}, \quad (49)$$

where the energies $E_{\infty, N}$ in the thermodynamic limit are

$$\frac{E_{\infty, N_a}}{N_a} = -2 \int_{-\pi}^{\pi} \rho_{\infty, N_a}(k) \cos k \, dk, \quad (50)$$

$$\frac{E_{\infty, N_a-2}}{N_a} = -2 \int_{-\pi}^{\pi} \rho_{\infty, N_a-2}(k) \cos k \, dk - \frac{4}{N_a}, \quad (51)$$

with $\rho_{\infty, N_a}(k)$ given by Eq. (35) and $\rho_{\infty, N_a-2}(k)$ by Eq. (39) with $k_h = \pm\pi$ and $\lambda_h = \pm\infty$.

Using Eqs. (47), (48), (46), (44), and Eq. (51) with ρ_{∞, N_a} and ρ_{∞, N_a-2} following from Eqs. (35) and Eq. (39), we obtain

$$\frac{\delta E_{N_a}}{N_a} = - \int_{-\pi}^{\pi} \epsilon_c(k) X_{N_a}^c(k) \, dk - \int_{-\infty}^{\infty} \epsilon_s(\lambda) X_{N_a}^s(\lambda) \, d\lambda, \quad (52)$$

$$\frac{\delta E_{N_a-2}}{N_a} = - \int_{-\pi}^{\pi} \epsilon_c(k) \tilde{X}_{N_a-2}^c(k) \, dk - \int_{-\infty}^{\infty} \epsilon_s(\lambda) X_{N_a-2}^s(\lambda) \, d\lambda, \quad (53)$$

where

$$\epsilon_c(k) = 2 \cos k + 2 \int_0^{\infty} \frac{J_1(\omega) \exp(-\omega u)}{\omega \cosh(\omega u)} \cos(\omega \sin k) \, d\omega, \quad (54)$$

$$\epsilon_s(\lambda) = 2 \int_0^{\infty} \frac{J_1(\omega)}{\omega \cosh(\omega u)} \cos(\omega \lambda) \, d\omega, \quad (55)$$

and we used the fact that $\epsilon_s(\pm\infty) = 0$, so that $\tilde{X}_{N_a-2}^s(\lambda)$ can be replaced by $X_{N_a-2}^s(\lambda)$ in Eq. (53).

For the repulsive Hubbard model at half filling, the gap is in the charge sector and the spin sector is gapless. Accordingly, the first term in the right-hand side of Eq. (52) describes the contribution of gapped charge excitations, and the second term is due to the contribution of gapless spin excitations.

We now return to Eq. (14) and using Eqs. (52), (53) write the finite size corrections to the gap of the attractive case in the form

$$\delta \Delta = \delta E_{N_a-2} - \delta E_{N_a} = \delta \Delta_{ng} + \delta \Delta_g + \delta, \quad (56)$$

where

$$\delta \Delta_{ng}/N_a = \int_{-\infty}^{\infty} \epsilon_s(\lambda) X_{N_a}^s \, d\lambda - \int_{-\infty}^{\infty} \epsilon_s(\lambda) X_{N_a-2}^s \, d\lambda, \quad (57)$$

is the contribution of the gapless sector,

$$\delta \Delta_g/N_a = \int_{-\pi}^{\pi} \epsilon_c(k) X_{N_a}^c \, dk - \int_{-\pi}^{\pi} \epsilon_c(k) X_{N_a-2}^c \, dk, \quad (58)$$

is due to gapped excitations, and we used a relation

$$\tilde{X}_{N_a-2}^c = X_{N_a-2}^c - \frac{1}{N_a} \sum_{h=1}^2 \delta(k - k_h) + \frac{1}{N_a} [\delta(k - \pi) + \delta(k + \pi)].$$

The term δ which is present in the gapped sector is given by

$$\delta = \sum_h \epsilon(k_h) - \epsilon(\pi) - \epsilon(-\pi) \quad (59)$$

and for $N_a \Delta_{\infty} \gtrsim 1$ it reduces to

$$\delta \approx \epsilon_c''(\pi) (k_h^+ - \pi)^2,$$

where k_h^+ is the value of k_h which is close to π at large N_a . This term behaves as $1/N_a^2$ for large N_a . In the limit of $u \ll 1$ the value of k_h^+ can be found from Eqs. (37) and (40) using the condition $Z_{N_a-2} = 1/2 - 1/2N_a$. For $N_a\Delta_\infty \gg 1$ we then obtain

$$\frac{\delta}{\Delta_\infty} = 2 \left(\frac{2\pi}{N_a\Delta_\infty} \right)^2, \quad (60)$$

where at half filling the gap of the thermodynamic limit Δ_∞ is given by

$$\Delta_\infty = 4u - 4 + 4 \int_0^\infty \frac{\exp(-\omega u) J_1(\omega)}{\omega \cosh \omega u} d\omega \quad (61)$$

at any interaction strength. As we will see below, the term δ (60) can become comparable with the (conformal) $1/N_a$ correction for $N_a\Delta_\infty \lesssim 40$ and exceeds higher order power law corrections up to much larger values of N_a .

Note that the contribution of the gapped charge excitations for the repulsive Hubbard model corresponds to the contribution of gapped spin excitations for the attractive model, and the contribution of gapless spin excitations corresponds to the contribution of gapless charge excitations in the attractive case.

The origin of the term δ is the following. The state with two additional or two missing spin-up (or spin-down) particles of the initial attractive Hubbard model contains unpaired fermions with energies above the gap. Gapped excitations of the model are $S = 1/2$ - solitons which appear only in pairs. We thus calculate the exact energy of the states with 2 solitons which have different nonzero momenta and energies near the bottom of the excitation band. The contribution (59) takes into account these nonzero kinetic energies of the solitons and is proportional to the curvature of the excitation spectrum.

It is worth noting that the term δ is independent of the definition of the gap, except for minor changes for a relatively small number of particles. For example, it remains the same (as well as all other results of our work) if we consider the gap in the spectrum of triplet excitations: $2\Delta = E(N/2 + 1, N/2 - 1, -|U|) - E((N/2, N/2, -|U|)$. In this case we just get two unpaired spin-up fermions.

The calculation for excited states of the system with unpaired fermions is the same as above. It simply assumes that k_h are no longer fixed by the condition $Z_c(k_h) = (N_a - 1)/2N_a$, but are related to the momenta $\pm p$ of the solitons. For the energy of the state containing two solitons with momenta p and $-p$ we have $\epsilon = 2\tilde{\Delta} + 2[\epsilon_c(\pi - p) - \epsilon_c(\pi)]$, and for low-lying excitations at sufficiently large number of particles it is reduced to $\epsilon = 2\tilde{\Delta} + \epsilon''(\pi)p^2$, where $\tilde{\Delta} = \Delta_\infty + \delta\Delta_{ng} + \delta_g$. The minimum value of ϵ is achieved at the minimum possible value of p which is equal to $(\pi - k_h^+)$, and we arrive at the gap $\Delta = \Delta_\infty + \delta\Delta$, with $\delta\Delta$ given by Eq.(56) and thus including δ (59). It is important that this Δ is just the gap that is measured by the radiospectroscopy method used for obtaining the gap in experiments with two-component 3D Fermi gases [9].

IV. EXPONENTIAL CORRECTIONS FOR HALF FILLING

Throughout the paper we discuss the case where the inequality

$$N_a u \gg 1 \quad (62)$$

is satisfied (except for Section VII), so that all analytical formulas obtained below remain valid for arbitrarily large N_a . It is convenient to present the results in terms of the parameters $N_a\Delta_\infty(u)$ and u because in the limit of $u \ll 1$ the most important contributions to both $\delta\Delta_g/\Delta_\infty$ and $\delta\Delta_{ng}/\Delta_\infty$ depend only on $N_a\Delta_\infty$ (see below).

In this Section we calculate the finite size corrections to the gap, originating from the gapped sector and given by Eq. (58). Using Eqs. (16), (29), (23) and the Poisson relation $\sum_m \delta(x - mn) = \sum_m \exp[2\pi x m i]$ we obtain

$$\int_{-\pi}^{\pi} \epsilon_c(k) X_N^c(k) dk = - \int_{-\pi}^{\pi} \epsilon_c(k) \left[\frac{\rho_N(k)}{\exp[-2\pi i N_a Z_N^c(k + i0)] + 1} + \frac{\rho_N(k)}{\exp[2\pi i N_a Z_N^c(k - i0)] + 1} \right] dk. \quad (63)$$

To lowest order, we take the functions $\rho_N(k)$ and $Z_N^c(k)$ equal to their values in the thermodynamic limit. So, they are given by Eq. (35) and Eq. (37) for the case $N = N_a$, and by Eq. (39) and Eq. (40) for $N = N_a - 2$, with $k_h = \pm\pi$ and $\lambda_h = \pm\infty$. One can show that the integral from $-\pi$ to π in the right -hand side of Eq. (63) is equal to the integral from $-\pi + i\text{arcsinh}u$ to $\pi + i\text{arcsinh}u$ for the first term of the integrand plus the integral from $-\pi - i\text{arcsinh}u$ to $\pi - i\text{arcsinh}u$ for the second term.

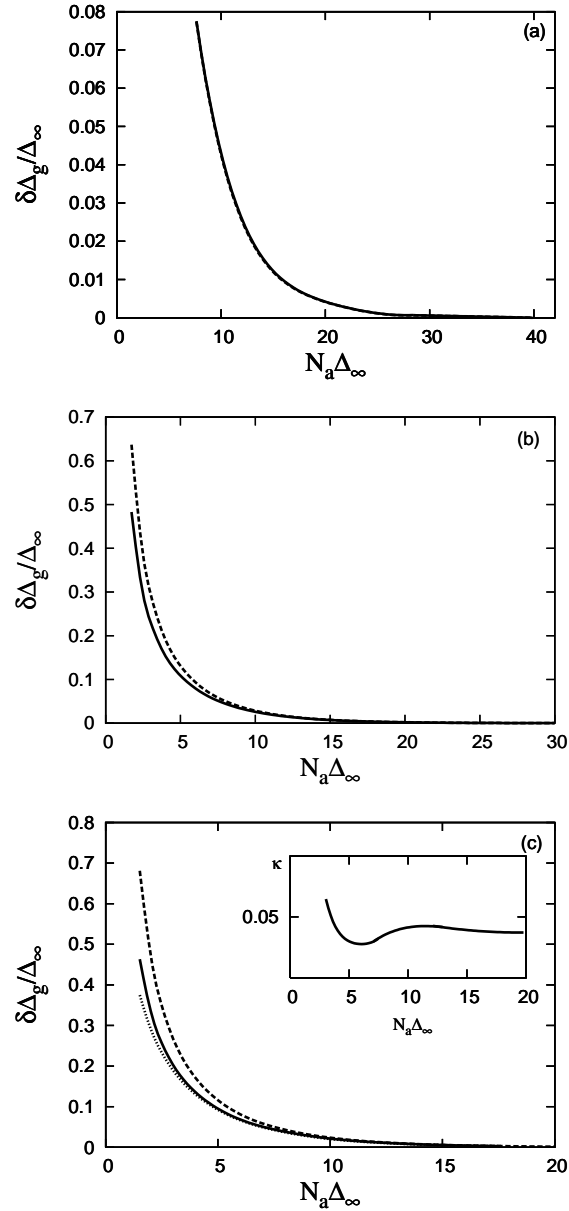


FIG. 1: The correction $\delta\Delta_g/\Delta_\infty$ versus $N_a\Delta_\infty$. The solid curve is the result of exact calculations from Eq. (58), and the dashed curve represents the result of Eq. (64). In a) $u = 1$, in b) $u = 0.5$, and in c) $u = 0.25$ with the dotted curve showing the result of Eq. (73), with the replacement $N_a \rightarrow N_a(1 - u/\pi)$ (see text after Eq. (73)). The inset in c) shows the relative difference between the exact $\delta\Delta_g$ and the exponential result of equation (73), $\kappa = (\delta\Delta_g^{\text{exact}} - \delta\Delta_g^{\text{exp}})/\delta\Delta_g^{\text{exact}}$.

Equation (58) then reduces to

$$\begin{aligned} \frac{\delta\Delta_g}{N_a} &= \int_{-\pi+i\gamma}^{\pi+i\gamma} \left[\frac{\rho_{N_a}(k)\epsilon_c(k)}{1 + \exp[-2\pi i N_a Z_{N_a}^c(k)]} - \frac{\rho_{N_a-2}(k)\epsilon_c(k)}{1 + \exp[-2\pi i N_a Z_{N_a-2}^c(k)]} \right] dk \\ &+ c.c. = \frac{1}{2\pi i N_a} \int_{-\pi+i\gamma}^{\pi+i\gamma} \epsilon'_c(k) \ln \left(\frac{1 + \exp[2\pi i N_a Z_{N_a}^c(k)]}{1 + \exp[2\pi i N_a Z_{N_a-2}^c(k)]} \right) dk + c.c., \end{aligned} \quad (64)$$

where $\gamma = \text{arcsinh}u$.

It is convenient to present the ratio $\delta\Delta_g/\Delta_\infty$ as a function of $N_a\Delta_\infty$ and u . In Fig. 1 we show $\delta\Delta_g/\Delta_\infty$ versus $N_a\Delta_\infty$ for several values of u , and one clearly sees that for not very large $N_a\Delta_\infty$ this correction becomes significant.

The edge points of the integration $k_0 = \pm\pi \pm i\text{arcsinh}u$ are the saddle points at which $\rho_{N_a}(k) = dZ_{N_a}/dk = 0$. For

sufficiently large N_a we may use the saddle point approximation, and the expression for $\delta\Delta_g$ becomes

$$\delta\Delta_g \approx C \frac{|\epsilon'_c(k_0)|}{\pi \sqrt{N_a} |\rho'(k_0)|} \exp[-S_0], \quad (65)$$

where

$$\epsilon'_c(k_0) = i \left[2u - 2\sqrt{u^2 + 1} \int_0^\infty J_1(\omega) \tanh(\omega u) \exp(-\omega u) d\omega \right], \quad (66)$$

$$\rho'(k_0) = \frac{i}{2\pi} \left[\frac{u}{\sqrt{u^2 + 1}} + (u^2 + 1) \int_0^\infty \omega \tanh(\omega u) J_0(\omega) \exp(-\omega u) d\omega \right], \quad (67)$$

$$S_0 = -2\pi i (Z_{N_a}^c(k_0) - 1/2) = N_a \left[\gamma - \int_0^\infty \frac{\tanh(\omega u) \exp(-\omega u)}{\omega} J_0(\omega) d\omega \right], \quad (68)$$

$$C = \left[1 - \left(\frac{\Gamma(3/4)}{2\Gamma(5/4)} \right)^4 \right], \quad (69)$$

and we used the relation

$$Z_{N_a-2}^c(k_0) = Z_{N_a}^c(k_0) + \frac{i}{\pi N_a} \int_0^\infty \frac{\tanh(\omega u)}{\omega} \exp(-\omega u) d\omega = Z_{N_a}^c(k_0) + \frac{2i}{\pi N_a} \ln \left[\frac{2\Gamma(5/4)}{\Gamma(3/4)} \right]. \quad (70)$$

The saddle point approximation assumes that the exponent in Eq. (65) is large:

$$S_0 \gg 1. \quad (71)$$

In the case of strong interaction, $u \gg 1$, Eq. (65) gives

$$\delta\Delta_g \approx \frac{1}{\sqrt{N_a} u^{N_a-1}}, \quad (72)$$

and one sees that in this limit the correction $\delta\Delta_g$ is negligible.

The situation changes for $u < 1$. In the limit of $u \ll 1$, from Eq. (65) we obtain:

$$\delta\Delta_g \approx C \sqrt{\frac{2}{\pi}} \frac{\Delta_\infty \exp[-\Delta_\infty N_a/4]}{\sqrt{\Delta_\infty N_a}} \approx 0.63 \frac{\Delta_\infty \exp[-\Delta_\infty N_a/4]}{\sqrt{\Delta_\infty N_a}}, \quad (73)$$

where the gap in the thermodynamic limit, Δ_∞ , is given by Eq. (11). The criterion (71) then becomes $N_a \Delta_\infty \gg 1$. The obtained relation (73) is in accordance with the universal scaling behavior of the gap in massive quantum field theories [19], which is expected for the Hubbard model at $u \ll 1$. For not very small u we should take into account corrections which are linear in u in the expression for S_0 and in the preexponential factor for Δ_∞ . This proves to be equivalent to the replacement $N_a \rightarrow N_a(1 - u/\pi)$ in Eq. (73). Higher order corrections become important only for $N_a \Delta_\infty$ which are so large that the exponential contribution $\delta\Delta_g$ is no longer important.

V. POWER LAW CORRECTIONS

The correction to the gap provided by the gapless sector, $\delta\Delta_{ng}$, we calculate using the conformal field theory $1/N_a$ expansion for the energy [11, 12, 13]:

$$E_{N_a} - E_0 = \frac{2\pi}{N_a} v_s (\Delta_+ + \Delta_-), \quad E_0 = \epsilon N_a - \frac{\pi}{6N_a} v_s, \quad (74)$$

where ϵN_a is the energy in the thermodynamic limit, and the velocity of spin excitations is given by

$$v_s = \frac{d\epsilon}{dp} = \frac{\epsilon'_s(B)}{2\pi\sigma(B)}, \quad (75)$$

where B is defined by Eq. (9). The conformal dimensions of primary operators are equal to

$$\Delta_\pm = \frac{1}{2} \left(\xi_s(B) D_s \pm \frac{\Delta N_s}{2\xi_s(B)} \right)^2. \quad (76)$$

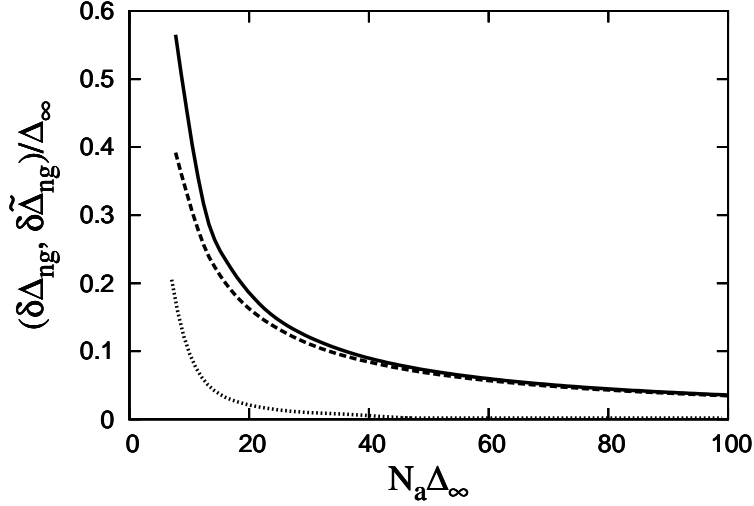


FIG. 2: The correction $\delta\Delta_{ng}/\Delta_\infty$ versus $N_a\Delta_\infty$ for $u = 1$. The solid curve shows the result of exact calculation from Eq. (57) and the dashed curve the result of Eq. (83). The dotted curve represents higher order power law corrections $\delta\tilde{\Delta}_{ng}$ (see text).

Integer or half-odd integer numbers ΔN_s , D_s are characterizing the excitation states. The component of the charge dressed matrix ξ_s is determined from the equation

$$\xi_s(\lambda) = 1 - \frac{1}{2\pi} \int_{-B}^B K_2(\lambda - \eta) \xi_s(\eta) d\eta. \quad (77)$$

For the zero-field case ($B = \infty$) the solution is $\xi_s = 1/\sqrt{2}$. The energy and momentum of a spin excitation are given by

$$\epsilon_s(\lambda) = 2 \int_0^\infty \frac{\cos \omega \lambda}{\cosh \omega u} J_1(\omega) \frac{d\omega}{\omega}, \quad (78)$$

$$p_s(\lambda) = \frac{\pi}{2} - \int_0^\infty \frac{\sin \omega \lambda}{\cosh \omega u} J_0(\omega) \frac{d\omega}{\omega}, \quad (79)$$

$$\frac{dp_s}{d\lambda} = -2\pi\sigma(\lambda). \quad (80)$$

The excitation state with the energy $E(N_a/2, N_a/2 - 2)$ is characterized by the numbers $D_s = 0$, $\Delta N_s = 1$. According to Eq. (14), this leads to the correction

$$\delta\Delta_{ng} = \frac{\pi}{2N_a} \frac{v_s}{\xi_s^2}. \quad (81)$$

For the half-filled case we obtain

$$\delta\Delta_{ng} = \frac{2\pi}{N_a} \frac{I_1(\pi/2u)}{I_0(\pi/2u)}. \quad (82)$$

A more accurate result following from the calculations in Refs. [11, 13] reads:

$$\delta\Delta_{ng} = \frac{2\pi}{N_a} \frac{I_1(\pi/2u)}{I_0(\pi/2u)} \left(1 - \frac{1}{2 \ln[N_a I_0(\pi/2u)]} \right). \quad (83)$$

The comparison of Eq. (83) with the result of exact calculations from Eq. (57) shows the validity of Eq. (83) even for not very large N_a (see Fig. 2). For example, at $u = 1$ even for $N_a = 10$ ($N_a\Delta_\infty \approx 13$) the relative difference is $\sim 20\%$. The subtraction of Δ_{ng} (83) from the exact result of Eq. (57) gives higher order power law corrections which we denote as $\delta\tilde{\Delta}_{ng}$. For $u = 1$ they are represented by the dotted curve in Fig. 2.

In the limit of strong coupling Eq. (82) yields:

$$\delta\Delta_{ng} \simeq \frac{\pi^2}{2N_a u}; \quad u \gg 1, \quad (84)$$

and the power law correction (84) always dominates over the negligible exponential correction (72). The situation changes for $u \lesssim 1$. For not very large $N_a\Delta_\infty$, the exponential correction $\delta\Delta_g$ originating from gapped excitations becomes comparable with $\delta\Delta_{ng}$ and exceeds higher order power law corrections. We provide a detailed comparison of Δ_g with power law corrections in the next section.

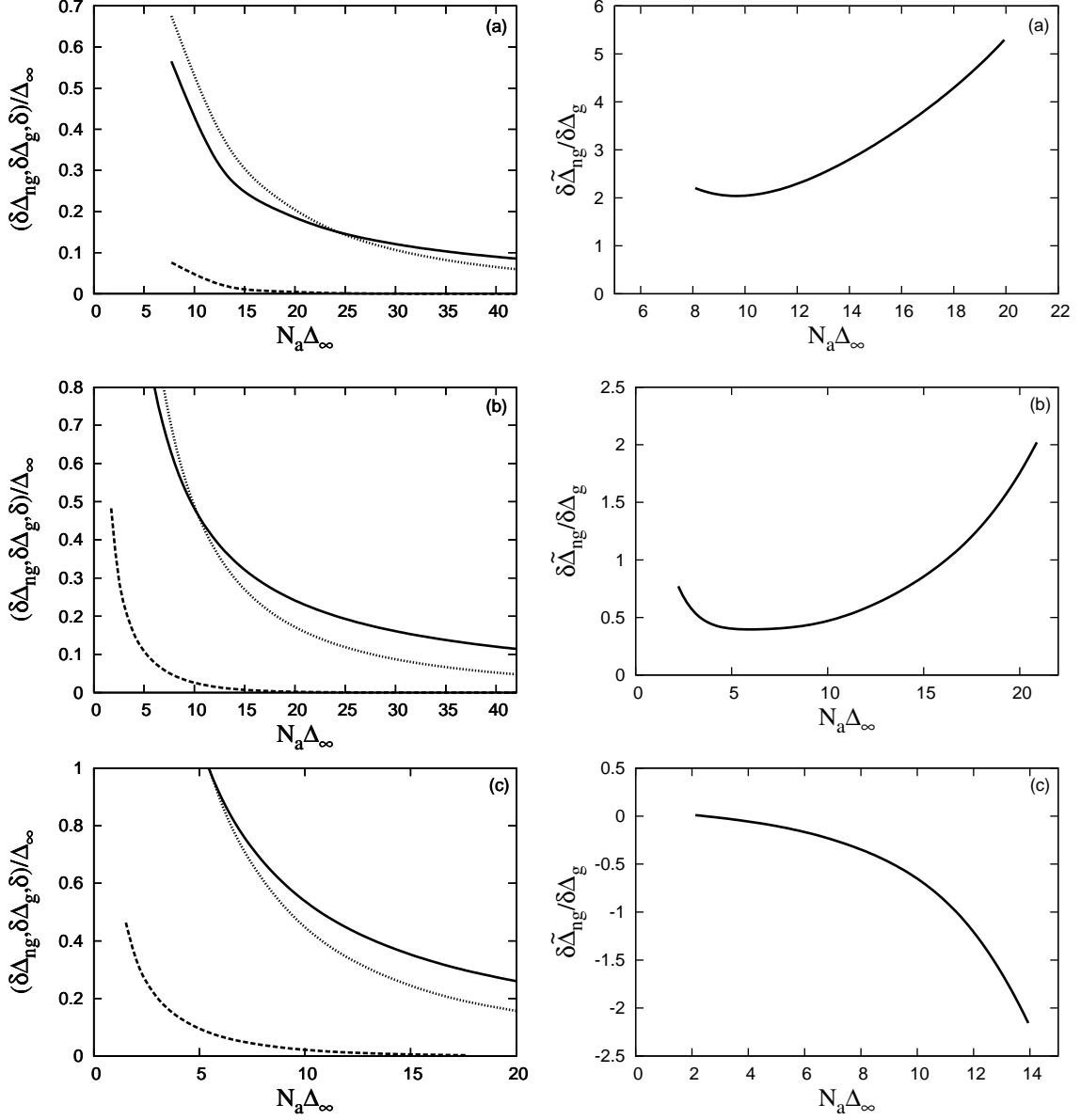


FIG. 3: The result of exact calculations from Eqs. (57), (58) and (59). In the left part the solid curve shows $\delta\Delta_{ng}/\Delta_\infty$ versus $N_a\Delta_\infty$, the dashed curve $\delta\Delta_g/\Delta_\infty$, and the dotted curve δ/Δ_∞ . In the right part the solid curve shows the ratio of the higher order power law corrections $\tilde{\delta\Delta}_{ng}$ to the exponential correction $\delta\Delta_g$. In a) $u = 1$, in b) $u = 0.5$, and in c) $u = 0.25$.

VI. DISCUSSION OF THE RESULTS

We start the comparison of the non-conformal exponential correction to the gap with power law corrections in the limiting case of $u \ll 1$ and $N_a \Delta_\infty \gg 1$, so that Eq. (73) is applicable. Then, comparing the result of Eq. (73) with that of Eq. (83) we see that the power law $1/N_a$ correction dominates over the exponential correction for any $N_a \Delta_\infty$ significantly larger than unity. However, the exponential correction (73) is still larger than higher order power law corrections in a wide range of N_a . In the limit of $N_a \rightarrow \infty$ the higher order corrections contain terms $\ln[\ln(N_a)]/(N_a \ln^q(N_a))$, $1/(N_a \ln^q(N_a))$, $1/N_a^2$, etc., where $q \geq 2$ is an integer [11]. Thus, for reasonable values of N_a the term that should be compared with $\delta\Delta_g$ (73) is $\sim 1/[N_a \ln^2(N_a)]$. The argument of the logarithm may contain an u -dependent multiple $B \sim \exp(\pi/2u)$ like the logarithm in the second term of Eq. (83). This is however not important. According to Eq. (11), in the limit of $u \ll 1$ the gap is exponentially small, $\Delta_\infty \sim \exp(-\pi/2u) \ll 1$. Hence, for N_a at which the exponential correction can still be important we have $N_a \Delta_\infty \ll \Delta_\infty^{-1}$ and $\ln(N_a) \approx \ln(\Delta_\infty^{-1}) \sim 1/u$. So, irrespective of the presence of the u -dependent multiple B , the higher order power law correction becomes $\sim (u^2/N_a) \ln(1/u)$ and it is smaller than the exponential correction (73) for N_a satisfying the inequality

$$N_a \Delta_\infty \lesssim 8 \ln\left(\frac{1}{u}\right); \quad u \ll 1. \quad (85)$$

Thus, at $u \ll 1$ for $N_a \Delta_\infty$ significantly larger than unity but still satisfying the condition (85), the exponential correction (73) is legitimate and can be kept together with the power law correction (83).

The situation is similar for intermediate values of u smaller than unity. This is seen from Fig. 3 where we present our numerical results for $u = 0.25$ and $u = 0.5$. However, already for $u = 1$ the exponential correction is smaller than the higher order power law terms (see Fig. 3) and should be omitted. As far as the term δ is concerned, for $u \ll 1$ it is comparable with the power law correction up to $N_a \Delta_\infty \sim 40$ and exceeds higher order power law corrections for much larger N_a . Even if we compare δ with the second term of Eq. (83), the latter is smaller at $N_a \Delta_\infty \lesssim 1/u$.

In Fig. 4 we present the results of exact calculations for the gap Δ at half filling from Eqs. (2), (3), (4) and (14) for the same u as in Fig. 3. A direct comparison of Δ with the gap of the thermodynamic limit Δ_∞ (61) shows that finite size corrections can be safely omitted for $N_a \Delta_\infty > 40$. On the other hand, already at $N_a \Delta_\infty < 10$, they dominate the gap. For $u = 0.25$ where $\Delta_\infty = 5 \cdot 10^{-3}$ this occurs already at $N_a < 1.5 \cdot 10^3$. For $u = 1$ we have $\Delta_\infty = 1.28$ and finite size corrections are important only for $N_a < 30$.

It is important that for $N_a \Delta_\infty \sim 10$ or even somewhat larger the non-conformal corrections originating from the gapped sector become comparable with power law corrections coming from the gapless sector. This is seen in Fig. 3. The exponential correction $\delta\Delta_g$ is about 20% of $\delta\Delta_{ng}$ or smaller, and the correction δ approaches $\delta\Delta_{ng}$ and can even exceed it.

Qualitatively, the dependence $\Delta(N_a)$ remains the same for smaller filling factors. This is seen from Fig. 5, where we present our numerical results for $n = 0.2$. For $u = 1$ finite size effects become important only at a very small number of lattice sites $N_a < 30$. For $u = 0.25$ the thermodynamic-limit gap is $\Delta_\infty \approx 6 \cdot 10^{-2}$ and finite size effects are already important for $N_a \approx 500$.

VII. LIMIT OF $N_a u \ll 1$

In the limit of $N_a u \ll 1$, which can be realized for $u \ll 1$, the energy spectrum of the attractive Hubbard Model shows no exponential gap and both charge and spin sectors are conformal. The analysis of Lieb-Wu equations for this case has been done in [20, 21], and found corrections $\sim u/N_a$. This can be understood from the conformal $1/N_a$ expansion as a consequence of the linear dependence of the velocities of elementary excitations on the interaction constant u [20, 22].

Here we consider the limit of $u N_a \ll 1$ for completeness and present first order corrections in u to the ground state energy and to the gap in the excitation spectrum. As in the previous sections, we calculate the energy for the Hubbard model in the repulsive case, where the Bethe Ansatz equations are easily solved, and then restore the energy for the attractive case using the particle-hole symmetry.

So, consider a system of N particles (N_\downarrow spin-down and $N - N_\downarrow$ spin-up) with repulsive interaction. From the Lieb-Wu equation (2) we obtain the momenta k_j to first order in u :

$$\exp(ik_j N_a) = \prod_{\alpha=1}^{N_\downarrow} \frac{\sin k_j - \lambda_\alpha + iu}{\sin k_j - \lambda_\alpha - iu} \Rightarrow \delta k_j = k_j - k_j^0 = \frac{1}{N_a} \sum_{\alpha=1}^{N_\downarrow} \frac{2u}{\sin(k_j^0) - \lambda_\alpha^0}, \quad (86)$$

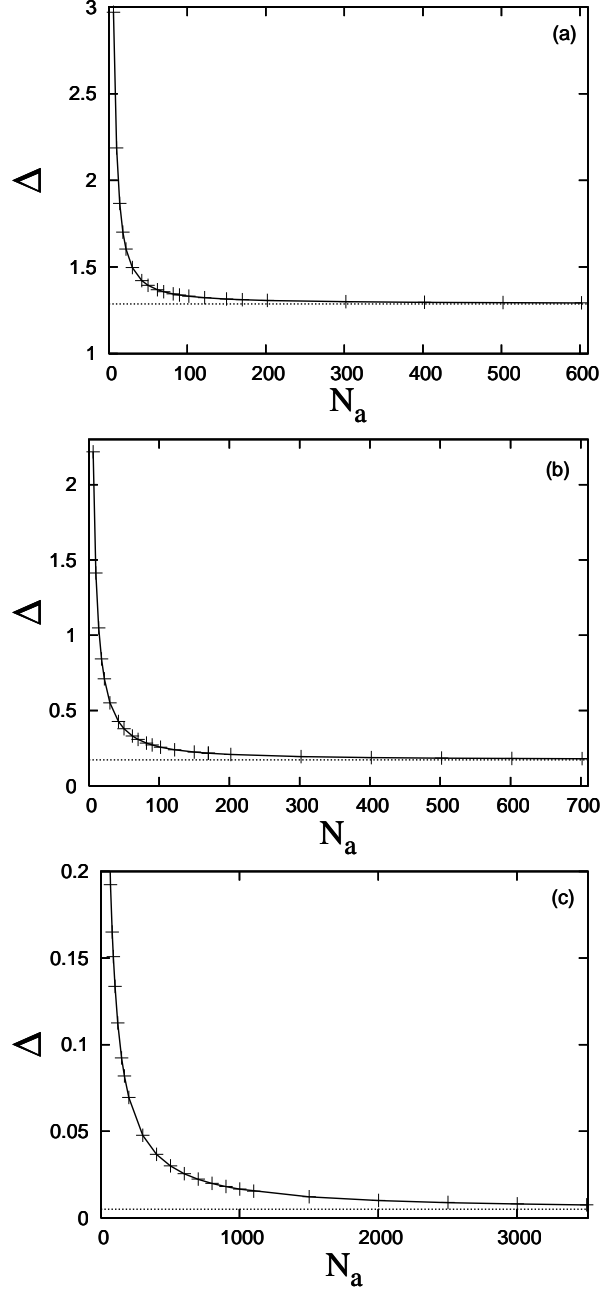


FIG. 4: The gap Δ in units of t versus N_a at half filling for $u = 1$ in a), $u = 0.5$ in b), and $u = 0.25$ in c). The dotted line is the value of the gap in the thermodynamic limit. The sum $\delta\Delta_{ng} + \delta\Delta_g + \delta + \Delta_\infty$ (solid curve) coincides with the value of the gap found directly (crosses) from the Bethe Ansatz equations (2) and (3) using Eqs. (4) and (14).

where k^0 and λ^0 are the momenta and rapidities for $u \rightarrow 0$. The energy itself and the interaction-induced change of the energy are given by

$$E = -2 \sum_{j=1}^N \cos k_j, \quad \delta E = E - E^0 = \frac{4u}{N_a} \sum_{j=1}^N \sum_{\alpha=1}^{N_\downarrow} \frac{\sin k_j^0}{\sin(k_j^0) - \lambda_\alpha^0}, \quad (87)$$

where E_0 is the ground state energy for $u \rightarrow 0$. We now calculate the densities of momenta k and rapidities λ in the

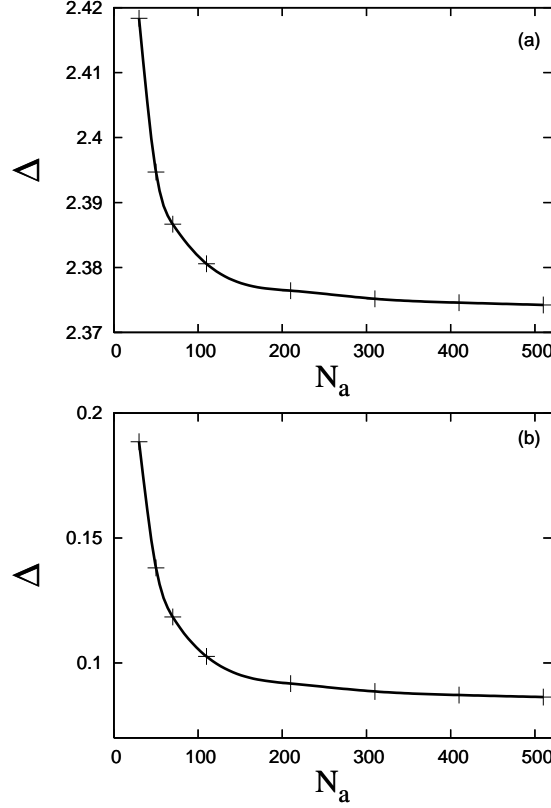


FIG. 5: The gap Δ in units of t versus N_a , calculated numerically for $u = 0.25$ in a), and $u = 1.25$ in b) for the filling factor $n = 0.2$.

thermodynamic limit from Eqs. (7) and (8). To the lowest order in u we obtain:

$$2\sigma(\lambda) = \int_{-Q}^Q \delta(\lambda - \sin k) \rho(k) dk, \quad (88)$$

$$\rho(k) = \frac{1}{2\pi} + \cos k \int_{-B}^B \delta(\lambda - \sin k) \sigma(\lambda) d\lambda. \quad (89)$$

The solution of Eqs. (88) and (89) is ($n_\downarrow \leq n_\uparrow$)

$$\rho(k) = \begin{cases} 1/\pi; & k \leq \pi n_\downarrow, \\ 1/2\pi; & \pi n_\downarrow < k \leq \pi(n - n_\downarrow). \end{cases} \quad (90)$$

$$\sigma(\lambda) = \frac{1}{2\pi} \frac{1}{\sqrt{1 - \lambda^2}}. \quad (91)$$

Then, using Eq. (9) for the total number of particles and the number of spin-down particles, we find an expression for the integration limits Q and B :

$$B = \sin(\pi n_\downarrow), \quad Q = \pi(n - n_\downarrow). \quad (92)$$

Using Eqs. (90) and (91) we obtain the interaction-induced change of the energy to first order in u :

$$\begin{aligned} \frac{\delta E}{N_a} &= 4u \int_{-Q}^Q dk \int_{-B}^B \frac{\sin k}{\sin k - \lambda} \sigma(\lambda) \rho(k) d\lambda = \\ &= \frac{4u}{\pi^2} (\pi n_\downarrow)^2 + \frac{4u}{\pi^2} \int_{\pi n_\downarrow}^{\pi(n - n_\downarrow)} dk \int_0^{\pi n_\downarrow} \frac{\sin^2 k}{\sin^2 k - \sin^2 q} dq, \end{aligned} \quad (93)$$

where we turned to the variable $q = \arcsin \lambda$. For the case of attraction we should substitute $n_\uparrow \rightarrow 1 - n_\uparrow$, $n_\downarrow \rightarrow n_\downarrow$, in accordance with the symmetry properties (12). Integrating over dq we find:

$$\frac{\delta E(-u)}{N_a} = -4un_\downarrow + 4un_\downarrow^2 + \frac{2u}{\pi^2} \left(2 \int_{\pi n_\downarrow}^{\pi/2} - \int_{\pi n_\downarrow}^{\pi n_\uparrow} \right) \tan k \ln \left(\frac{\tan k + \tan \pi n_\downarrow}{\tan k - \tan \pi n_\downarrow} \right) dk, \quad (94)$$

where n_\downarrow and n_\uparrow are already occupation numbers for the attractive Hubbard model, and we assume that $n_\downarrow \leq n_\uparrow$. Eq. (94) leads to the following result for the interaction-induced change of the energy to first order in $N_a u$:

$$\begin{aligned} \frac{\delta E(-u)}{N_a} &= 4un_\downarrow^2 - 4un_\downarrow + \frac{4u}{\pi} \arctan \pi n_\downarrow - \frac{u}{\pi^2} \ln \left(\frac{1 + \tan^2 \pi n_\uparrow}{1 + \tan^2 \pi n_\downarrow} \right) \ln \left(\frac{\tan \pi n_\uparrow + \tan \pi n_\downarrow}{\tan \pi n_\uparrow - \tan \pi n_\downarrow} \right) \\ &+ \frac{2u}{\pi^2} \left(-\operatorname{Re} Li_2 \left(\frac{2 \tan \pi n_\downarrow}{\tan \pi n_\downarrow - i} \right) - \operatorname{Re} Li_2 \left(\frac{\tan \pi n_\uparrow + \tan \pi n_\downarrow}{\tan \pi n_\downarrow - i} \right) + \operatorname{Re} Li_2 \left(\frac{\tan \pi n_\uparrow - \tan \pi n_\downarrow}{-\tan \pi n_\downarrow - i} \right) \right), \end{aligned}$$

where $Li_2(z) = \sum_{k=1}^{\infty} z^k/k^2$ is a polylogarithmic function.

In the limit of small filling factors, $N_\uparrow \ll N_a$ and $N_\downarrow \ll N_a$, after a straightforward algebra we obtain:

$$\frac{\delta E}{N_a} \approx u(-4n_\downarrow - 4n_\uparrow n_\downarrow + 2n_\downarrow^2) \quad (95)$$

The limit of small filling factors in the Hubbard model corresponds to the gas phase of spin-1/2 fermions. For this case the ground state energy at $Nu \ll 1$ has been calculated in Refs. [16, 17, 18], and the result of Eq. (95) coincides with that of Refs. [16, 17, 18] in the attractive case.

Using Eq. (6) we then find a small interaction-induced correction to the gap in the excitation spectrum ($n_\uparrow = n_\downarrow = n/2$) of the attractive model to the lowest order in uN_a . For small filling factors we have: $\delta\Delta \approx 4u/N_a$, and in the considered limit of $N_a u \ll 1$ this correction is small compared to the level spacing $\sim 1/N_a$ in our finite size system.

VIII. CONCLUSIONS

In conclusion, we have studied finite size effects for the gap in the excitation spectrum of the 1D Fermi Hubbard model with one-site attraction. For the situation in which the thermodynamic-limit gap Δ_∞ exceeds the level spacing (near the Fermi energy) of the finite size system, there are two types of finite size corrections. For large interactions ($u \gg 1$) the leading is a power law conformal correction to Δ_∞ , which behaves as $1/N_a$ and originates from the gapless sector of the excitation spectrum. We also find non-conformal corrections originating from the gapped branch of the spectrum. As found at half filling, in the weakly interacting regime ($u \lesssim 1$) the non-conformal corrections can become of the order of the conformal correction even for the number of particles (lattice sites) as large as $\sim 20/\Delta_\infty$. Also, for $u \ll 1$ and large $N_a \Delta_\infty$, the exponential correction (73) is legitimate as long as the condition (85) is satisfied. Thus, we have the full right to take it into account together with the power law correction (83).

For sufficiently small number of lattice sites (particles) the gap Δ is dominated by finite size effects. From a general point of view, this happens when $\Delta_\infty \lesssim 1/N_a$, i. e. Δ_∞ is smaller than the level spacing of the finite size system at energies close to the Fermi energy. Accordingly, for large interactions ($u \gg 1$) the finite size effects are not important as long as $N_a \gg 1$. However, in the weakly interacting regime ($u \lesssim 1$) they become dominant already at significantly larger N_a than a simple dimensional estimate $1/\Delta_\infty$. This is clearly seen from our results in Fig. 3 and Fig. 4 for $\Delta(N_a)$ at half filling.

Our findings are especially important for the studies of the 1D regime with cold atoms, where the number of particles in a 1D tube ranges from several tens to several hundreds [6, 7]. For such a system in the weakly interacting regime one can not use the result of the thermodynamic limit for the gap. Consequently, one can not employ the local density approximation for Δ based on this result, for finding the spectrum of isospin gapped excitations in an external harmonic potential.

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