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Correlation Functions and Coulomb Blockade of Interacting Fermions at Finite Temperature and Size

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Abstract

We present explicit expressions for the correlation functions of interacting fermions in one dimension which are valid for arbitrary system sizes and temperatures. The result applies to a number of very different strongly correlated systems, including mesoscopic quantum wires, quantum Hall edges, spin chains and quasi-one-dimensional metals. It is for example possible to calculate Coulomb blockade oscillations from our expression and determine their dependence on interaction strength and temperature. Numerical simulations show excellent agreement with the analytical results.

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Recently, there has been great interest in strongly correlated systems of all kinds, which is spurred by high temperature superconductivity, progress in mesoscopic physics, quantum Hall systems, and newly available materials which accurately display the characteristics of one-dimensional metals or spin chains. In the case of quasi-one-dimensional electron systems much progress can be made with the Luttinger liquid formalism [1] which is able to describe virtually any type of local interaction and can be solved by use of bosonization techniques [2,3]. Using these methods, it is well known how to calculate correlation functions in the infinite length or zero temperature limit and therefore determine the spectral properties [4] of a number of systems, like mesoscopic quantum wires, quantum Hall bars [5], quasi one-dimensional metals and spin chains [6,7] even in the presence of boundaries [8,9]. We now present explicit expressions for the correlation functions which are valid at arbitrary temperature, system size, and distances (as long as the lattice spacing is relatively small). These expressions can be used to calculate Coulomb blockade oscillations in mesoscopic systems as a function of the interaction strength and of temperature. Monte Carlo simulations of one of the simplest systems, namely interacting spinless fermions on a one-dimensional lattice, show excellent agreement with our result.

As our model Hamiltonian we consider one-dimensional interacting fermions in the continuum limit

$$H \;=\; \int_0^\ell dx \quad \left[v_F \; \psi_L^\dagger i \frac{d}{dx} \psi_L - v_F \; \psi_R^\dagger i \frac{d}{dx} \psi_R \;+\; g_1 (J_L J_L \;+\; J_R J_R) \;+\; g_2 J_L J_R \right] \tag{1}$$

Here $J_{L/R} \equiv \, :\psi_{L/R}^\dagger \psi_{L/R}:$ are the chiral fermion currents of the left- and right-moving components of the fermion field $\Psi(x)$, expanded about the Fermi points $\pm k_F$, $\Psi(x) = e^{-ik_F x}\psi_L(x) + e^{ik_F x}\psi_R(x)$. This expansion is valid as long as the lattice spacing a is small compared to the inverse temperature $v\beta$ and the length scales we want to consider. In this limit the Hamiltonian (1) can describe almost any one-dimensional fermion system with short range interactions by choosing appropriate coupling constants g_1 and g_2. The umklapp process $e^{i4k_F x} \; \psi_L^\dagger \psi_R \psi_L^\dagger \psi_R + h.c.$ can also be included, but it only contributes if the system is close to half-filling $k_F = \pi/2a$ and then it can often be absorbed by renormalizing the coupling constant g_2 [1].

The fermion correlation functions of systems with the Hamiltonian of equation (1) are known to obey simple power-laws in the zero-temperature and infinite length limit, with exponents determined by the interaction [1]. At non-zero temperatures the correlation functions are exponentially damped and are described by powers of the hyperbolic sine in the infinite length limit. For finite length ℓ and periodic boundary conditions, on the other hand, the correlation functions are periodic and at zero temperature are described by powers of the sine instead. The correlation functions are essential to understand the spectral characteristics and other properties of experimental systems, and it is often necessary to consider both finite size and finite temperature. We will now derive explicit expressions for this case and show the crossover between the two limits.

To establish notation we will review shortly the bosonization formalism [3] for the Hamiltonian (1), which is given by the relations

$$J_{L,R} = \frac{1}{4\pi}\partial_x(\phi \pm \tilde{\phi}), \qquad \psi_{L,R} \propto e^{-i\sqrt{\pi}(\tilde{\phi}\pm\phi)} \tag{2}$$

where $\tilde{\phi}$ is the dual field to the boson ϕ with the finite length mode expansion

$$\phi(x,t) = \phi_0 + \Pi\frac{vt}{\ell} + Q\frac{x}{\ell} + \sum_{n=1}^{\infty}\frac{1}{\sqrt{4\pi n}}\left[e^{-\frac{2\pi i}{\ell}n(vt+x)}a_n^L + e^{-\frac{2\pi i}{\ell}n(vt-x)}a_n^R + h.c.\right]$$
$$\tilde{\phi}(x,t) = \tilde{\phi}_0 + Q\frac{vt}{\ell} + \Pi\frac{x}{\ell} + \sum_{n=1}^{\infty}\frac{1}{\sqrt{4\pi n}}\left[e^{-\frac{2\pi i}{\ell}n(vt+x)}a_n^L - e^{-\frac{2\pi i}{\ell}n(vt-x)}a_n^R + h.c.\right]. \qquad (3)$$

Here Π and Q are canonically conjugate to the zero modes ϕ_0 and $\tilde{\phi}_0$, respectively, and the time variable implicitly carries a small ultraviolet cutoff $t - i\alpha$.

The g_1 interaction can be absorbed by redefining the velocity $v = v_F + g_1/2\pi$, and the Hamiltonian density becomes

$$\mathcal{H} = \frac{v}{2}\left[(\partial_x\phi)^2 + (\partial_x\tilde{\phi})^2\right] + \frac{g_2}{4\pi}\left[(\partial_x\phi)^2 - (\partial_x\tilde{\phi})^2\right]. \qquad (4)$$

The Hamiltonian is then solved by a simple rescaling of the boson,

$$\phi \to K\phi, \quad \tilde{\phi} \to \tilde{\phi}/K, \qquad (5)$$

where $K = 1 - g_2/4\pi v$ to lowest order in the coupling constant (i.e. $K = 1$ for a non-interacting system and $K < 1$ for repulsive interactions).

The eigenvalues of the operators Π and Q are quantized by using the relation for periodic boundary conditions $\psi_{R,L}(0,t) = e^{\pm ik_F\ell}\psi_{R,L}(\ell,t)$ together with equations (2) and (3). After a careful consideration of the commutation relations we find

$$Q = \sqrt{\pi}(n - n_0)/K, \quad \Pi = \sqrt{\pi}Km, \qquad (6)$$

where n and m are either both even or both odd integers and $n_0 = \frac{k_F\ell}{\pi} + 1$ which can be defined modulo 2. The quantum number n represents the particle number and m is a measure of the current in the ring. If a magnetic field is applied, the ground state may have quantum number $m \neq 0$ and the system carries a persistent current [10,11].

As a simple example of our calculation at finite temperature and size, we now want to consider the chiral Green's function

$$G(x,t) \equiv \left\langle \psi_L(x,t)\psi_L^\dagger(0,0)\right\rangle \qquad (7)$$

but the generalization to more complicated correlation functions is straightforward as we will see later. Using equations (2) and (5) and applying the Baker-Hausdorf formula as well as the cumulant theorem for bosonic modes, we obtain

$$G(x,t) \propto \left\langle \exp -i\sqrt{\pi}\left[K\phi(x,t) + \tilde{\phi}(x,t)/K\right]\exp i\sqrt{\pi}\left[K\phi(0,0) + \tilde{\phi}(0,0)/K\right]\right\rangle \qquad (8)$$
$$= e^{-i\frac{\pi}{\ell}[x + \frac{K^2+1/K^2}{2}vt]}\, B(x,t)\, \exp\left[\pi(K + K^{-1})^2 G_L(x,t)\right]\exp\left[\pi(K - K^{-1})^2 G_R(x,t)\right]$$

where $B(x,t) \equiv \left\langle \exp -i\sqrt{\pi}\left(Q\frac{Kx+vt/K}{\ell} + \Pi\frac{Kvt+x/K}{\ell}\right)\right\rangle$ is the contribution from the operators Π and Q, and $G_{L,R} \equiv \left\langle \phi_{L,R}(x,t)\phi_{L,R}(0,0) - \phi_{L,R}^2(0,0)\right\rangle$ are the chiral boson Green's functions for the left- and right-moving modes $\phi_{L,R} = [\phi \pm \tilde{\phi} - (Q \pm \Pi)\frac{x \pm vt}{\ell}]/2$, respectively. Using the mode expansion (3) the chiral boson Green's function can be expressed as

$$G_L(x,t) \;=\; \frac{1}{4\pi}\sum_{n=1}^{\infty}\frac{1}{n}\left[(e^{-i2\pi n\frac{x+vt}{\ell}}-1)\left\langle a_n^L a_n^{L\dagger}\right\rangle + (e^{i2\pi n\frac{x+vt}{\ell}}-1)\left\langle a_n^{L\dagger} a_n^L\right\rangle\right]. \tag{9}$$

Since we know the energy levels $E_n = n\frac{2\pi v}{\ell}$ of the free boson modes, it is useful to write the Bose-Einstein distribution as a sum over occupation numbers $\left\langle a_n^\dagger a_n\right\rangle = \frac{1}{e^{\beta E_n}-1} = \sum_{k=1}^{\infty} e^{-\frac{2\pi v}{\ell}\beta k n}$. After exchanging the order of the summations over k and n we can use the identity $\sum_{n=1}^{\infty}\frac{x^n}{n} = -\ln(1-x)$ to obtain

$$G_L(x,t) \;=\; -\frac{1}{4\pi}\ln\left[\frac{1-e^{-2\pi i(x+vt)/\ell}}{\pi\alpha/\ell}\prod_{k=1}^{\infty}\frac{1-e^{-2\pi i(x+vt-iv\beta k)/\ell}}{1-e^{-2\pi v\beta k/\ell}}\frac{1-e^{2\pi i(x+vt+iv\beta k)/\ell}}{1-e^{-2\pi v\beta k/\ell}}\right] \tag{10}$$

Using the elliptic theta function of the first kind $\theta_1(z,q)$ [12], this result can be written more compactly as

$$G_L(x,t) = i\frac{x+vt}{4\ell} - \frac{1}{4\pi}\ln\frac{\theta_1(\pi\frac{x+vt}{\ell}, e^{-\pi v\beta/\ell})}{\theta_1(-i\frac{\pi\alpha}{\ell}, e^{-\pi v\beta/\ell})} \tag{11}$$

and likewise for $G_R(x,t) = G_L(-x,t)$.

The cumulant theorem does not apply to the contribution $B(x,t)$ from the operators Π and Q, but we can use the energy spectrum $E = \frac{v}{2\ell}(Q^2+\Pi^2)$ and sum over all eigenvalues in equation (6). The result can again be expressed in terms of the elliptic theta functions [12]

$$B(x,t) = e^{in_0 x_Q}\frac{\theta_2(x_Q + i\gamma\frac{n_0}{K^2}, e^{-2\gamma/K^2})\theta_2(x_\Pi, e^{-2\gamma K^2}) + \theta_3(x_Q + i\gamma\frac{n_0}{K^2}, e^{-2\gamma/K^2})\theta_3(x_\Pi, e^{-2\gamma K^2})}{\theta_2(i\gamma\frac{n_0}{K^2}, e^{-2\gamma/K^2})\theta_2(0, e^{-2\gamma K^2}) + \theta_3(i\gamma\frac{n_0}{K^2}, e^{-2\gamma/K^2})\theta_3(0, e^{-2\gamma K^2})} \tag{12}$$

where $\gamma \equiv \frac{\pi v\beta}{\ell}$ is a measure of the energy gap compared to the temperature scale, and we have defined $x_Q \equiv \frac{\pi}{\ell}(x + vt/K^2)$ and $x_\Pi \equiv \frac{\pi}{\ell}(x + vtK^2)$. The complete chiral Green's function therefore reduces to a compact expression

$$G(x,t) \propto B(x,t)\left[\frac{\theta_1(\pi\frac{x+vt}{\ell}, e^{-\pi v\beta/\ell})}{\theta_1(-i\frac{\pi\alpha}{\ell}, e^{-\pi v\beta/\ell})}\right]^{-(K+\frac{1}{K})^2/4}\left[\frac{\theta_1(\pi\frac{vt-x}{\ell}, e^{-\pi v\beta/\ell})}{\theta_1(-i\frac{\pi\alpha}{\ell}, e^{-\pi v\beta/\ell})}\right]^{-(K-\frac{1}{K})^2/4}. \tag{13}$$

We can immediately verify that this expression is anti-periodic under translation $t \to t + i\beta$ and periodic under translation $x \to x + \ell$ up to a phase of $e^{ik_F\ell}$ as it should be.

If the temperature is much smaller than the energy gap of the system, i.e. $\gamma = \frac{\pi v\beta}{\ell} \to \infty$, we can use the limits of the theta function [12] as $q = e^{-\gamma} \to 0$ to find

$$G(x,t) \to e^{i(n_0 \bmod 2)x_Q}\left[\frac{\ell}{\pi}\sin(\pi\frac{x+vt}{\ell})\right]^{-(K+\frac{1}{K})^2/4}\left[\frac{\ell}{\pi}\sin(\pi\frac{vt-x}{\ell})\right]^{-(K-\frac{1}{K})^2/4} \tag{14}$$

which is the expected finite length result [1]. For special values of n_0 the overall phase may have a different x-dependence, which will not be discussed here in detail.

Likewise, we can explore the limit of a large system size compared to the temperature scale, i.e. $\gamma \to 0$. We use the Poisson summation formula to find $\theta_1(z, e^{-\gamma}) \approx 2\sqrt{\frac{\pi}{\gamma}} e^{-z^2/\gamma} e^{-\pi^2/4\gamma} \sinh\frac{\pi z}{\gamma}$ and $\theta_2(z, e^{-\gamma}) \approx \theta_3(z, e^{-\gamma}) \approx \sqrt{\frac{\pi}{\gamma}} e^{-z^2/\gamma}$ as $e^{-\gamma} \to 1$ so that the correct finite temperature result [13] is reproduced

$$G(x,t) \to \left[\frac{v\beta}{\pi}\sinh(\pi\frac{x+vt}{v\beta})\right]^{-(K+\frac{1}{K})^2/4} \left[\frac{v\beta}{\pi}\sinh(\pi\frac{vt-x}{v\beta})\right]^{-(K-\frac{1}{K})^2/4} . \tag{15}$$

Taking the limit $l \to \infty$ in equation (14) or $v\beta \to \infty$ in equation (15) recovers the well known universal power-laws.

One interesting aspect of equations (12) and (13) is the dependence on the variable $n_0 = \frac{k_F \ell}{\pi} + 1$. The Green's function (13) is invariant under the increase of n_0 by 2, i.e. periodic in k_F with period $\frac{2\pi}{\ell}$. Hence, as we change the Fermi energy (e.g. by applying a gate voltage), the spectral properties of the system are changed periodically. These are Coulomb blockade oscillations [15,16], which come from the fact that the system has a regular energy-level spacing. In the case of Luttinger liquids this level spacing has been derived from a complete solution of a quantum system which takes all interactions into account and cannot be obtained from a geometrical analysis of the capacitance as in the usual quantum-dot systems. As possible experimental setups to test this periodicity we can imagine electron tunneling through a quasi one-dimensional wire or ring of mesoscopic size. Such wires can be fabricated by etching, gating [17] or by cleaved edge overgrowth [18]. A small gated quantum hall bar on the other hand should exhibit *chiral* Luttinger liquid behavior which can be examined with the same formalism, except that in that case the rescaling parameter K is fixed by the filling fraction in the bulk of the quantum Hall bar [5]. The experimental situation is developing quickly and most recently carbon nanonubes have been produced which were seen to exhibit the charactersitcs of one dimensional wires [19].

As an example we consider the Green's function at the lowest Matsubara frequency $i\omega_0 = i\pi/\beta$ for spin-less Fermions on a ring. This quantity only gives an indirect indication of experimental tunneling resonances, but it is a simple illustration of the properties of equation (13) as a function of temperature and interaction. The absolute value of the Matsubara Green's function has been plotted in figure (1) as a function of the Fermi wave-vector in arbitrary units. As the Fermi-level is changed, the system shows periodic resonances which become more pronounced as the temperature is lowered. These peaks occur at special values of $n_0 = \frac{1+K^4}{2}$, $\frac{3-K^4}{2}$ where the even and odd sectors of n and m in equation (6) give the same degenerate ground state. Hence, the spacing of the resonances can give a direct experimental measure of the interaction strength K [11]. As shown in the inset of figure (1) a non-interacting system ($K = 1$) has only one central peak in the range $0 \leq n_0 < 2$, while an interacting system has two split resonances. The physical interpretation of the resonances is that tunneling of an extra electron into the system does not require any additional energy at the degenerate values of n_0 so that such processes are enhanced. Recently, much progress has also been made with Bethe ansatz methods [14], which showed evidence of Coulomb-blockade-like oscillations in a strongly interacting system, but in contrast to statements made in that paper, field theoretical methods also predict the desired Coulomb blockade oscillations [15,16]. Using our result (13) it is now possible to determine the complete spectral properties, including the dependence of the Coulomb blockade oscillations on interactions and on temperature for any of the systems mentioned above.

So far we have taken the fermion field to be spinless, but the results apply equally well to electrons with spin because the well known spin-charge separation allows the same formalism to be used for the spin and the charge excitations separately [1]. It is also well understood how to incorporate open boundary condition within the same formalism [9,20].

To test our result, we will now consider one of the simplest models of spinless interacting fermions described by the Hamiltonian

$$H = -t \sum_x \left[\psi^\dagger(x)\psi(x+1) + h.c.\right] + U \sum_x \left[n(x) - \frac{1}{2}\right]\left[n(x+1) - \frac{1}{2}\right], \tag{16}$$

where $n = \psi^\dagger\psi$, and the lattice constant has been set to unity. In this case the coupling constants are given by $g_1 = g_2/4 = U$. We have chosen the system to be at half-filling $k_F = \pi/2$ where the model is equivalent to the xxz spin chain. In this case the umklapp process is allowed, but irrelevant, and the rescaling parameter K and the velocity v can actually be determined exactly by comparison with Bethe ansatz results [21], i.e. to all orders in the coupling constants. For our numerical simulations we have taken $t = U$ which corresponds to $K^2 = \frac{3}{4}$ and $v = t\frac{3\sqrt{3}}{2}$. In particular, we consider the equal time density-density correlation function $\langle n(x)n(0)\rangle$. At half filling the density-density correlation function acquires an alternating part which dominates the uniform contribution and can be expressed in terms of chiral fermions

$$\langle n(x)n(0)\rangle_{\mathrm{alt}} \propto e^{2ik_F x}\left\langle \psi_L^\dagger(x)\psi_R(x)\psi_R^\dagger(0)\psi_L(0)\right\rangle. \tag{17}$$

Following the analogous steps from equation (8) to equation (13) we find

$$\langle n(x)n(0)\rangle_{\mathrm{alt}} \propto (-1)^x \left|\frac{\theta_1(\frac{\pi x}{\ell}, e^{-\gamma})}{\theta_1(\frac{i\pi\alpha}{\ell}, e^{-\gamma})}\right|^{-3/2} \frac{\theta_2(\frac{2\pi x}{\ell}, e^{-8\gamma/3})\theta_3(0, e^{-3\gamma/2}) + \theta_3(\frac{2\pi x}{\ell}, e^{-8\gamma/3})\theta_2(0, e^{-3\gamma/2})}{\theta_2(0, e^{-8\gamma/3})\theta_3(0, e^{-3\gamma/2}) + \theta_3(0, e^{-8\gamma/3})\theta_2(0, e^{-3\gamma/2})}. \tag{18}$$

Here we took n_0 to be odd, i.e. ℓ divisible by four, but other cases have similar expressions.

For comparison we performed numerical Monte Carlo simulations using the Hamiltonian (16) and extracted the alternating part of the density-density correlation function to determine the unknown proportionality constant in equation (18). This prefactor should be independent of x up to corrections for smaller distances, which come from irrelevant terms in the Hamiltonian that can be neglected in the long-distance limit $x \gg \alpha$. As shown in figure (2) the prefactor is indeed constant within the error-bars of the Monte Carlo simulations for all system sizes ℓ and temperatures. This serves as a very sensitive test of our theoretical predictions since the expression (18) varies over several orders of magnitude over the range shown, so that even slight changes from the predicted expression (18) would have resulted in huge deviations from a constant for larger values of x. Using the previously known approximate expressions (14) or (15) is not sufficient in this case.

We therefore conclude that our field theoretical calculations make very accurate estimates for the correlation functions of almost any one-dimensional interacting system at arbitrary temperature and system size (as long as the cutoff α is small compared to the corresponding scales). The results can be used to determine the complete spectral behavior of such systems, including Coulomb blockade oscillations as a function of both interaction and temperature. Monte Carlo simulations serve as accurate "experiments", which confirm the results.

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FIGURES

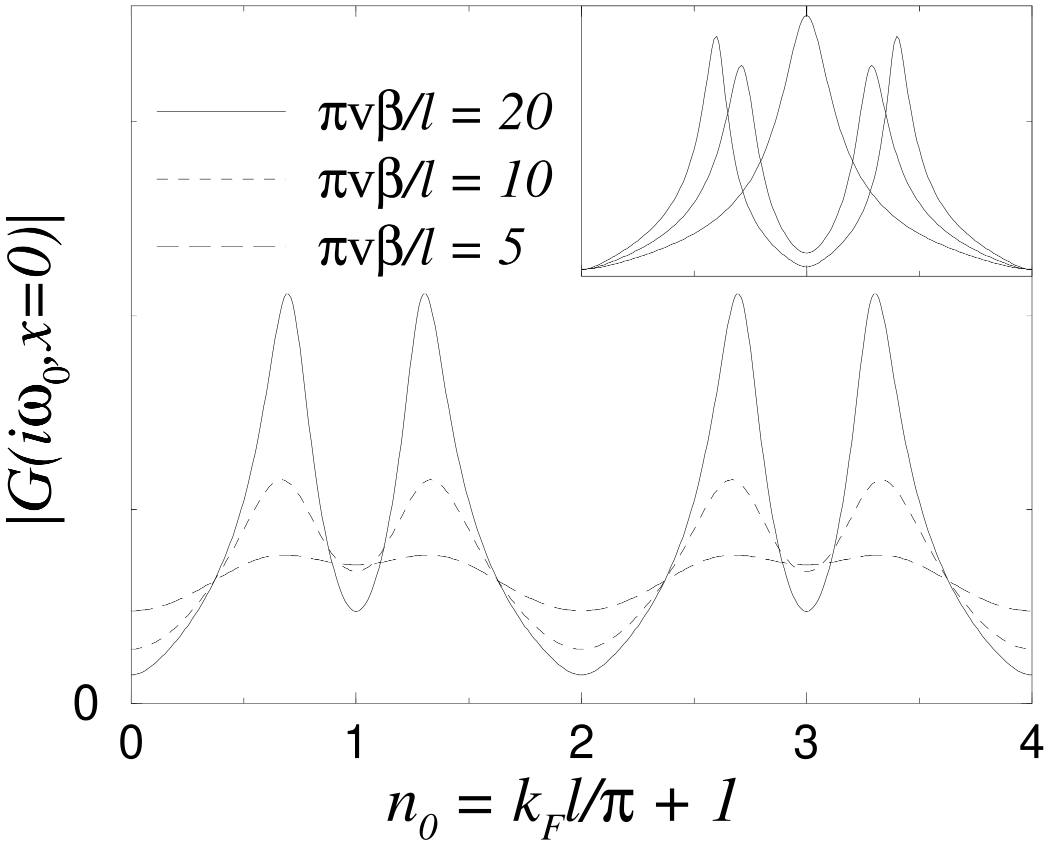

FIG. 1. The absolute value of the Green's function at the Matsubara frequency $i\omega_0 = i\pi/\beta$ as a function of the Fermi wave-vector k_F for different temperatures and $K^2 = 0.7$. The periodic resonances in the spectral properties are the so-called Coulomb blockade oscillations. The inset shows the curves for different interaction parameters $K^2 = 0.5,\ 0.7,\ 1$ at $\frac{\pi v \beta}{l} = 30$.

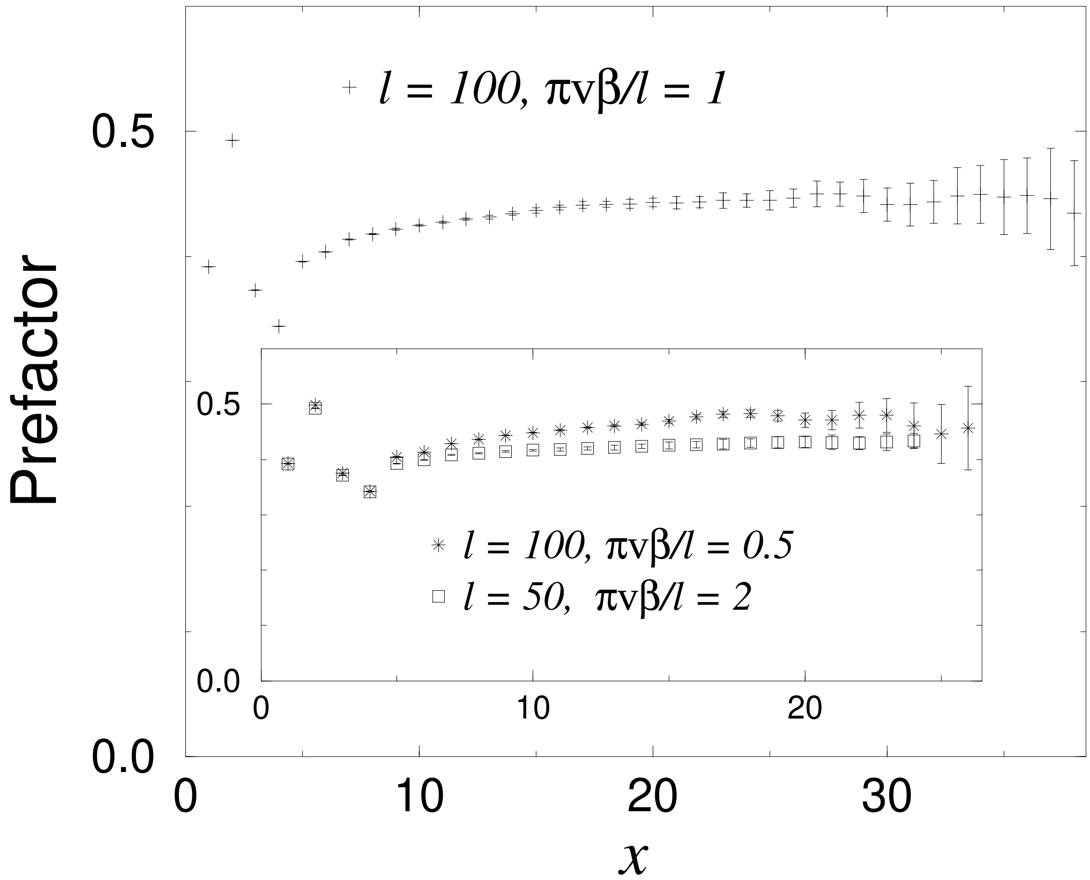

FIG. 2. The prefactor of equation (18), which is determined by dividing the alternating part of the density-density correlations from numerical simulations by the expressions of equation (18) for each correlation length x separately. As predicted, the prefactor is asymptotically constant in all cases.