Evaluation of the two-particle propagator for the Hubbard model with the help of the Hubbard-I approximation

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Received 6 October 2010, in final form 5 December 2010
Published 20 January 2011
Online at stacks.iop.org/JPhysCM/23/065601

Abstract
The Hubbard-I approximation is generalized to allow for direct evaluation of the equal-time anomalous two-electron propagator for the Hubbard model on a two-dimensional square lattice. This propagator is compared against the quantum Monte Carlo data obtained by Aimi and Imada (2007 J. Phys. Soc. Japan 76 113708) in the limit of strong electron–electron interaction. The Hubbard-I predictions are in good qualitative agreement with the Monte Carlo results. In particular, d-wave correlations decay as $cr^{-3}$ (‘free-electron’ behaviour) if the separation $r$ exceeds 2–3 lattice constants. However, the Hubbard-I approximation underestimates the coefficient $c$ by a factor of about 3. We conclude that the Hubbard-I approximation, despite its simplicity and artefacts, captures the qualitative behaviour of the two-particle propagator for the Hubbard model, at least for moderate values of $r$.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

1.1. General outlook

Consider the Hubbard model Hamiltonian [1]:

$$H = H_{\text{kin}} + H_{\text{int}} - \mu \sum_{i,\sigma} n_{i\sigma},$$

where

$$H_{\text{kin}} = -t \sum_{i,\sigma,\bar{\sigma}} c_{i\sigma}^\dagger c_{i\bar{\sigma}}^\sigma, \quad H_{\text{int}} = U \sum_i n_{i\sigma} n_{i\bar{\sigma}}.$$  (2)

Here $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron with spin projection $\sigma$ on site $i$ of the square lattice, $t$ is the hopping integral, $U$ is the on-site Coulomb repulsion, $\mathbf{a}$ are vectors connecting the site $i$ with its nearest neighbours, $\mu$ is the chemical potential, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the electron number operator, and $\bar{\sigma}$ means not $\sigma$.

This Hamiltonian is commonly used to describe systems of strongly correlated electrons. Among these, we mention such important examples as high-$T_c$ superconducting cuprates, manganites, cobaltites, etc. However, there is no commonly accepted method that allows us to solve the Hubbard model for a generic value of the doping.

One of the most intriguing problems as regards the Hubbard model is the question of whether the model captures the essential physics of the high-temperature copper oxide superconductors. At low interaction one expects the model to exhibit Kohn–Luttinger superconductivity [2–5]. Unfortunately, the critical temperature in such a regime is very small. Thus, it is necessary to study the Hubbard model at moderate or large interaction strengths. Such a regime is tractable only when the concentration of electrons is low [6–8]. However, the electron concentration for all known copper oxide superconductors is close to one electron per unit cell. Little rigorous knowledge is available for this limit. Different approaches return quite controversial answers: some Monte Carlo (MC) studies argue against superconductivity [9], or against high-$T_c$ superconductivity [10] in the Hubbard model; other numerical works favour the existence of a superconducting ground state with high condensation energy [11].

In the moderate and strong coupling limits there is no guidance from analytical studies either: in this parameter region the majority of theoretical methods become unreliable. Thus, one is forced to utilize uncontrollable devices with unknown accuracy.
In such a situation it appears useful to investigate the reliability of uncontrollable schemes. A particularly convenient uncontrollable approach for the analysis of the Hubbard model is that using the Hubbard-I approximation [1]. The Hubbard-I approximation, being invalid for $U \lesssim zt$ (where $z$ is the number of the nearest neighbour sites on the lattice), could be considered as a good first approximation in the case of strong correlations $U \gg zt$. Its evident advantage is its simplicity. The method allows deriving analytical results in many cases or performing numerical calculations at low computational cost.

The clarity and transparency of the Hubbard-I approximation explains its popularity among the researchers working in the field of strongly correlated electronic systems. For us, it is especially important that, since the discovery of high-$T_c$ superconductors, the method has been applied to superconductivity as well. Namely, the Hubbard-I approximation is used for the study of superconductivity in the Hubbard or extended Hubbard model [12, 13], in the Hubbard model with phonons [14–16], and in the Hubbard model with attractive interaction [17, 18]. A related approach, that using the two-pole approximation (which, in some respects, is superior to the Hubbard-I approximation), and its generalization are applied to study possible superconductivity of the usual Hubbard model [19] and of the multi-band Hubbard model [20]. Similar techniques are used in [21, 22]. Systematic expansion in orders of $t/U$ is developed in [23]. This contains the Hubbard-I approximation as a special case.

1.2. Our results

Despite broad use of the Hubbard-I approximation, its ability to account for superconducting properties is untested. In this paper we address this issue by comparing the Cooper pair propagator found with the help of generalized Hubbard-I method against the same propagator calculated within the MC framework (in this paper we refer to our calculations to account for superconducting properties is untested. In section 2 we derive the equation of motion for the two-particle propagator. The numerically calculated Hubbard-I correlation function is presented and compared against the Monte Carlo data in section 3. The results obtained are discussed in section 4.

2. The Hubbard-I approximation

2.1. The general idea

The idea of the Hubbard-I approximation for Hamiltonian (1) is as follows. First, we introduce the single-electron Matsubara Green’s function $G_\sigma(j - i, \tau) = -\langle \hat{T}_\tau \delta(j + a, \tau) \rangle$, where $\langle \cdots \rangle$ means the thermodynamic average, $T$ is the time-ordering operator, and $\tau$ is imaginary time. The equation of motion for $G_\sigma(j - i, \tau)$ can be written as

$$
\begin{align*}
-\frac{\partial}{\partial \tau} + \mu & \quad G_\sigma(j - i, \tau) = \delta_\delta(\tau) + UF_{\sigma\bar{\sigma}}(j - i, \tau) \\
& \quad - t \sum_a G_\sigma(j - i + a, \tau),
\end{align*}
$$

(3)

where $\delta_\delta$ is the Kronecker symbol, $\delta(\tau)$ is the delta function, and $F_{\sigma\bar{\sigma}}(j - i, \tau)$ is the two-particle Green’s function of the form

$$
F_{\sigma\bar{\sigma}}(j - i, \tau) = -\langle \hat{T}_\tau c_{j\sigma}^\dagger(\tau) n_{j\bar{\sigma}}(\tau) c_{k\bar{\sigma}}(0) \rangle.
$$

(4)

Second, we write the equation of motion for the function $F$, which includes even more complicated Green’s functions, which, in turn, require additional equations of motion, etc. In the Hubbard-I approximation we avoid proliferation of these Green’s functions by carrying out the following decoupling:

$$
\langle \hat{T}_\tau c_{j+a\sigma}(\tau) n_{j\bar{\sigma}}(\tau) c_{k\bar{\sigma}}(0) \rangle \to \langle n_{j\bar{\sigma}} \rangle \langle \hat{T}_\tau c_{j+a\sigma}(\tau) c_{k\bar{\sigma}}(0) \rangle,
$$

(5)

$$
\langle \hat{T}_\tau c_{j\sigma}(\tau) c_{j+a\sigma}^\dagger(\tau) c_{j\bar{\sigma}}(\tau) c_{k\bar{\sigma}}(0) \rangle \to \langle c_{j\sigma} c_{j\bar{\sigma}} \rangle \langle \hat{T}_\tau c_{j+a\sigma}^\dagger(\tau) c_{k\bar{\sigma}}(0) \rangle = 0,
$$

(6)

$$
\langle \hat{T}_\tau c_{j \sigma}(\tau) c_{j+a\sigma}^\dagger(\tau) c_{k \bar{\sigma}}(\tau) c_{k \bar{\sigma}}(0) \rangle \to \langle c_{j \sigma} c_{\bar{\sigma}}^\dagger \rangle \langle \hat{T}_\tau c_{j+a\sigma}^\dagger(\tau) c_{k \bar{\sigma}}(0) \rangle = 0.
$$

(7)

To understand the nature of this approximation let us express the electron density as a sum of its average value and fluctuations around it:

$$
n_{j\bar{\sigma}} = \langle n_{j\bar{\sigma}} \rangle + \delta n_{j\bar{\sigma}}, \quad \text{where}
$$

$$
\delta n_{j\bar{\sigma}} = n_{j\bar{\sigma}} - \langle n_{j\bar{\sigma}} \rangle.
$$

(8)

(9)

Two other boson-like quantities, $c_{j\bar{\sigma}} c_{j\bar{\sigma}}^\dagger$ and $c_{j\bar{\sigma}} c_{j\bar{\sigma}}^\dagger$, can be represented in the same manner. The above decouplings correspond to the assumption that the propagation of a single electron is unaffected by the fluctuations of these quantities around their average values. This assumption could be proven by showing either that (i) the fluctuation terms were small or...
that (ii) there were no correlation between the single-electron motion and the fluctuations. Unfortunately, neither (i) nor (ii) is rigorously established. Because of this the Hubbard-I approximation is an uncontrollable approach whose accuracy is unknown.

Using the decouplings (5)–(7) we derive the equation for \( F \) in the form

\[
\left(-\frac{\partial}{\partial \tau} + \mu - U\right) F_{0\delta}(j-1, \tau)
= \langle n_{\delta j} \rangle \left[ \delta_{ij} \delta(\tau) - t \sum_{a} G_{a}(j - 1 + a, \tau) \right].
\]

This equation, together with (3), constitutes a closed system, sufficient for the calculation of functions \( G \) and \( F \). This is how the single-electron propagator is calculated within the framework of the Hubbard-I approximation.

2.2. The Hubbard-I approximation for the two-particle propagator

Following [10], we calculate here the equal-time two-electron correlation functions of the form

\[
P_{d}(r) = \frac{1}{2N} \sum_{i=1}^{N} (\Delta_{\delta}(i) \Delta_{0}(i + r) + \Delta_{\delta}(i) \Delta_{0}(i + r)),
\]

where \( N \) is the number of sites on the square lattice,

\[
\Delta_{\delta}(i) = \frac{1}{\sqrt{2}} \sum_{r} f_{d}(r) \left( \Delta_{i + r} + \Delta_{i + r} \right),
\]

\[
\Delta_{\deltaij} = c_{i}^{\dagger} c_{j}^{\dagger}.
\]

The form factor

\[
f_{d}(r) = \delta_{r,0} \left( \delta_{r,1} + \delta_{r,-1} \right) - \delta_{r,0} \left( \delta_{r,1} + \delta_{r,-1} \right)
\]

corresponds to the \( \delta \) wavelet order parameter.

To calculate \( P_{d}(r) \) let us first define the propagator

\[
P_{dijm}(\tau) = \langle \hat{T} \Delta_{\delta ij}(\tau) \Delta_{0lm}(0) \rangle.
\]

The equal-time two-electron correlation function \( P_{d}(r) \) is related to \( P_{dijm}(\tau) \) as follows:

\[
P_{d}(r) = \frac{1}{4N} \sum_{\text{hbo}} f_{d}(b) f_{d}(b') \left[ P_{i+\text{h},i+r,1,1+1}^{+}(\tau) + P_{i+\text{h},i+r,1,1+1}^{+}(\tau) + P_{i+\text{h},i+1+r,1}^{+}(\tau) \right]_{\rightarrow \leftarrow +0, \: r \rightarrow -r}.
\]

We write down the equation of motion for the propagator \( P_{dijm}(\tau) \) using Hamiltonians (1) and (2) as such

\[
\left(-\frac{\partial}{\partial \tau} + 2\mu\right) P_{dijm} = -t \sum_{a} \left( P_{i+\text{aljm}}^{+} + P_{ij+l+\text{am}}^{+} \right) + \delta(\tau) \left( c_{i}^{\dagger} c_{j}^{\dagger} \delta_{jm} - c_{m}^{\dagger} c_{p}^{\dagger} \right) \delta_{il} + \tau P_{dijm},
\]

where the three-particle propagator is defined as

\[
P_{dijm}(\tau) = \langle \hat{T} \Delta_{\delta ij}(\tau) n_{\delta j}(\tau) + n_{\delta j}(\tau) \Delta_{\delta ij}(\tau) \Delta_{0lm}(0) \rangle.
\]

Double occupancy is very unlikely: \( P_{ijlm}^{0} = o(\tau/U) \approx 0 \) if \( i = j \) or \( i = m \). Assuming the absence of magnetic order, which means, in particular, \( \langle c_{i}^{\dagger} c_{j}^{\dagger} c_{j}^{\dagger} c_{i}^{\dagger} \rangle = \langle c_{i}^{\dagger} c_{j}^{\dagger} c_{j}^{\dagger} c_{i}^{\dagger} \rangle \), we transform (16) in the Hubbard-I approximation to

\[
\left(-\frac{\partial}{\partial \tau} + 2\mu\right) P_{dijm} = -t \sum_{a} \left( P_{i+\text{aljm}}^{+} + P_{ij+l+\text{am}}^{+} \right) \left( 1 - \delta_{i+a}^{+} \right)
+ \delta(\tau) \left( c_{i}^{\dagger} c_{j}^{\dagger} \delta_{jm} - c_{m}^{\dagger} c_{l}^{\dagger} \right) \delta_{il} + \tau P_{dijm}.
\]

This relation is derived under the assumption that the magnetic order is absent: \( \langle n_{\delta j} \rangle = \langle n_{\delta i} \rangle \).

Substituting (19) in (18), we obtain the equation of motion for the propagator \( P_{dijm} \) in the Hubbard-I approximation valid when \( i \neq j \) and \( i \neq m \):

\[
\left(-\frac{\partial}{\partial \tau} + 2\mu\right) P_{dijm} = -t \sum_{a} \left( P_{i+\text{aljm}}^{+} + P_{ij+l+\text{am}}^{+} \right) \left( 1 - \delta_{i+a}^{+} \right)
+ \delta(\tau) \left( c_{i}^{\dagger} c_{j}^{\dagger} \delta_{jm} - c_{m}^{\dagger} c_{l}^{\dagger} \right) \delta_{il} + \tau P_{dijm}.
\]

Here \( \tau = (1 - \langle n_{\delta j} \rangle) \) if the system is uniform. As noted above, \( P_{dijm} \sim o(\tau/U) \approx 0 \) within our accuracy. Thus, jumps from site \( j = 1 + a \) to site \( m \) is excluded. The same is true for jumps from \( i = j + a \) to \( j \). To take this fact into account and to generalize the last equation for the case \( i = j \), we add the term \( t \sum_{a} \left( 1 - \langle n_{\delta j} \rangle \right) \delta_{ij} \delta_{jm}^{+} \delta_{il}^{+} \delta_{il} \) to the right-hand side of (20). Therefore

\[
\left(-\frac{\partial}{\partial \tau} + 2\mu\right) P_{dijm} = -t \sum_{a} \left( P_{i+\text{aljm}}^{+} + P_{ij+l+\text{am}}^{+} \right) \left( 1 - \delta_{i+a}^{+} \right)
+ \delta(\tau) \left( c_{i}^{\dagger} c_{j}^{\dagger} \delta_{jm} - c_{m}^{\dagger} c_{l}^{\dagger} \right) \delta_{il} + \tau P_{dijm}.
\]

In such an equation the quantity \( P_{dijm} \) is decoupled from \( P_{dijm} \), \( i \neq j \), which is equivalent to the condition \( P_{dijm} = 0 \).

Expression (21) corresponds to the propagation of two interacting particles: the terms with the Kronecker symbols may be regarded as an effective repulsive interaction between electrons on neighbouring sites with a coupling constant of the order of \( t \) (1 - \( \langle n_{\delta j} \rangle \)). Thus, we reduce the strong coupling many-body problem to the intermediate coupling two-body one.

3. Numerical results

3.1. The Hubbard-I approach versus the MC approach

In this section we present the results of our numerical calculation of the equal-time two-electron correlation function (10) at a given doping level. The actual calculations are based on
The doping level can be adjusted by changing $\mu$. For calculations at zero temperature it is convenient to use a substitution in (C.4):

$$N_0(\varepsilon) = \frac{1}{\sinh(\varepsilon/T)} - n_F(\varepsilon).$$

At $T = 0$ the Fermi distribution function is zero (unity) for $\varepsilon > 0$ ($\varepsilon < 0$). The contribution from $1/\sinh(\varepsilon/T)$ vanishes at low temperature.

Numerical results are shown in figures 1 and 2, where the propagator is plotted versus separation $r = |r|$ on the log–log graph. The Hubbard-I propagator $P_{\text{HI}}$ is shown as the dashed (blue) line. For comparison, the same propagator computed by Aimi and Imada [10] using the assumption-free quantum Monte Carlo procedure, $P_{\text{MC}}$, is shown by the solid (red) line. The subscript ‘HI’ stands for ‘Hubbard-I’, the subscript ‘MC’ for ‘Monte Carlo’.

In figure 1 we present the Hubbard-I data calculated for a $10 \times 10$ lattice for the doping level of 0.17. The same lattice size is used in the MC simulation of [10]. The MC data are collected for the doping level of 0.18. The small discrepancy in the densities is unavoidable in our situation.

Indeed, due to the finite size of the system, the number of particles cannot be changed continuously. In addition, in the case of the Hubbard-I scheme, the number of physical electrons is not an independent quantity, but rather has to be calculated according to formula (24). Given these two circumstances, it is impossible in general to match the MC and Hubbard-I densities exactly. However, such a small discrepancy (less than 6%) is of little importance for our goal.

The solid straight line fits the MC propagator in the window $0.32 < \log_{10} r < 0.78$. Such a fit corresponds to $c/r^3$ decay, as discussed in [10]. Propagator $P_{\text{HI}}$ is also fitted by a straight line (the blue/dashed straight line) in the window $0.3 < \log_{10} r < 0.6$.

To extract the asymptotic behaviour of $P_{\text{HI}}(r)$ more reliably it is better to look at the propagator on a bigger lattice. In figure 3 it is shown how the propagator converges for large lattices. We observe that the curves for the lattices with $M \geq 20$ almost coincide for moderate $r$. Thus, such systems can be used to find the asymptotics. To that end, let us examine figure 2. It presents the Hubbard-I data for a $28 \times 28$ lattice shown together with the MC data. Analysis of figure 2 reveals that the difference between assumption-free MC and much simpler Hubbard-I calculations is not large; moreover, the qualitative appearances of the curves are similar. In particular, both curves decay as a power law, $c/r^3$. In [10] it is established that $\nu \approx 3$, which is consistent with the free-electron behaviour. To determine this exponent for the Hubbard-I correlation function we use a two-parameter least-square fitting procedure for the Hubbard-I data in the range $0.3 < \log_{10} r < 0.9$. Fitting returns the following values:

$$\log_{10} c_{\text{FIT}} = -1.2 \pm 0.1, \quad \nu_{\text{FIT}} = 3.1 \pm 0.2. \quad (26)$$

The value of $\nu_{\text{FIT}}$ is consistent with the MC result. Below we will always assume that the Hubbard-I correlation function decays with $\nu \approx 3$. Deviations from the free-electron behaviour at large $r$ are a manifestation of the finite-size effects.
Indeed, in the latter equation, if \( \alpha \) and the doping close to 0.18 are plotted. While the curve for the window 0
\[
\log_{10}(P) /
\log_{10}(r)
\]
aim we fit both functions in figure 2 with straight lines in the
\[
\text{which correspond to }
\]
data by eliminating ‘noise’ in the propagators with the help of
\[
\text{the assumption-free Monte Carlo method within an order of}
\]
Hubbard-I propagator’s asymptotic form coincides with the
\[
c
\]
for lattices of three different sizes (16 × 16, 20 × 20, and 28 × 28)
Finite-size scaling for the Hubbard-I propagator: the data
\[
\text{Figure 3.}
\]
is a rather simple consequence of the equation of motion, (21).
\[
\text{The fact that the MC propagator decays like the free-}
\]
electron propagator is a surprising revelation of [10]. The
\[
\text{The ability of the Hubbard-I approximation to capture the }
\]
1/r^3 law is a rather simple consequence of the equation of motion, (21). Indeed, in the latter equation, if \( r \) is large, the interaction terms (the terms with the Kronecker symbols) contribute to the s-wave channel only; as for the d-wave propagator, its equation
\[
\text{of motion coincides, up to a normalization factor, with that for}
\]
free fermions.
In figure 2 the values obtained for the propagators are ‘noisy’. These oscillations arise because, in general, the propagators depend not only on the distance \( r \), but also on the direction of the vector \( \mathbf{r} \). Despite the ‘noise’, one can readily observe that the Hubbard-I propagator \( P_{\text{HI}} \) is smaller than the
\[
\text{Monte Carlo propagator } P_{\text{MC}}.
\]
To examine \( P_{\text{HI}} \) and \( P_{\text{MC}} \) in a more rigorous manner let us quantify the 1/r^3 behaviour of the propagators. With this aim we fit both functions in figure 2 with straight lines in the window 0.32 < log_{10} \( r \) < 0.78. The fit lines are defined by the equations
\[
\log_{10} P_{\text{MC}} = -0.81 - 3 \log_{10} r, \quad (27)
\]
\[
\log_{10} P_{\text{HI}} = -1.29 - 3 \log_{10} r, \quad (28)
\]
which correspond to \( P_{\text{HI}}(r) \approx \frac{c_{\text{HI}}}{r^3} \) with \( c_{\text{MC}} \approx 0.15 \), \( c_{\text{HI}} \approx 0.051 \), and the ratio \( c_{\text{MC}}/c_{\text{HI}} \approx 2.9 \). Thus, the Hubbard-I propagator’s asymptotic form coincides with the asymptotic form of the propagator calculated with the help of the assumption-free Monte Carlo method within an order of magnitude, but, of course, not exactly.
We can further compare the Hubbard-I and Monte Carlo data by eliminating ‘noise’ in the propagators with the help of the following procedure. Define the sum
\[
I(r) = \sum_{\sqrt{x^2+y^2} < r} P_{\text{s}}(x, y). \quad (29)
\]
If we assume that \( P_{\text{s}}(x, y) \sim c(\phi)r^{-3} \), where \( \phi \) is the polar angle, then \( I(r) \) can be approximated as
\[
I(r) \approx \int_{x^2+y^2 < r^2} dx \, dy \, P(x, y) \approx \alpha - \frac{\beta}{r}, \quad (30)
\]
where
\[
\beta = \int_0^{2\pi} c(\phi) \, d\phi = 2\pi \tilde{c}, \quad (31)
\]
and the constant \( \alpha \) can be estimated as \( \alpha \approx I(r_{\text{max}}) \), with \( r_{\text{max}} = M/2 \). Function \( I(r) \), by its definition, is independent of vector \( \mathbf{r} \)’s direction. Consequently, it is a smooth function, free from the irregular oscillations present in figure 2. This makes the fitting procedure more robust.
The dependence of \( \log_{10}(\alpha - I) \) versus \( \log_{10} r \) is plotted in figure 4 for the same values of parameters as for the data in figure 2. Like for the data presented in figure 3, the 16 × 16 curve lies somewhat away from the curves corresponding to the larger lattices. The curves for the 20 × 20 and 28 × 28 lattices coincide with each other almost everywhere, suggesting that for systems of such sizes the finite-size effects are important for large \( r \) only.
To determine the asymptotic parameters the curves in figure 4 are fitted with the straight lines
\[
\log_{10}(\alpha - I) = \log_{10} 2\pi \tilde{c} - \log_{10} r. \quad (32)
\]
The values of the fitting constants are \( \tilde{c}_{\text{MC}} \approx 0.15 \), \( \tilde{c}_{\text{HI}} \approx 0.055 \). As expected, they are close to \( c_{\text{MC}} \) and \( c_{\text{HI}} \).

3.2. Application
The numerical procedure in the case of the Hubbard-I approximation is much simpler than the quantum Monte Carlo computations. One can use it to derive different properties of the Hamiltonian (2). As an example, we apply the Hubbard-I approximation (B.10) to calculate the equal-time two-electron correlation function in the s channel:
\[
P_s(r) = \frac{1}{2N} \sum_{i=1}^{N} \langle \Delta_s(i) \Delta_s(i + r) + \Delta_s(i) \Delta_s^*(i + r) \rangle, \quad (33)
\]
The result is shown in figure 5 by the solid (red) line. The function $P_s(r)$ decays quickly for small $r$. At larger $r$ it oscillates around finite-value plateau. As could be expected, the s-wave superconducting correlations are weaker and decay faster than the d-wave ones (compare the solid (red) and dashed (green) lines in figure 5). This is because the electrons in the s channel experience strong repulsion, suppressing the superconducting correlations.

Note also that the Hubbard-I correlation functions show no sign of superconducting instability in either s or d channels: both correlation functions decay at large $r$, while in a superconducting phase the order parameter correlation function must saturate at large distances.

**4. Discussion**

We calculated the two-electron equal-time d-wave propagator using the Hubbard-I approximation and compared the results with quantum Monte Carlo computations [10]. The results from the two approaches are in good qualitative agreement. Specifically, both methods predict that the correlation function decays as $1/r^3$ at $r$ exceeding several lattice constants. This allows us to assess the reliability of the Hubbard-I approximation.

Technically speaking, the $1/r^3$ decay of the Hubbard-I propagator is a consequence of the fact that the interaction in the equation of motion, (21), is important in the s channel only, whereas in the d channel its effect decreases when $r$ increases. The Hubbard-I approximation underestimates the value of the propagator residue by a factor of order 3. Such a discrepancy is reasonable for an uncontrollable approach.

Our results for the two-particle correlation functions suggest that the Fermi liquid is a poor approximation for the Hubbard model near half-filling. We show that in the d-wave channel the correlation function decays as $r^{-3}$, which is consistent with ‘free fermions’. However, fast decay of the s-wave propagator (see figure 5) does not agree with the Fermi liquid picture. One must, however, remember that, unlike the d-wave propagator, the Hubbard-I s-wave correlation function is not compared against a controllable method; thus, its accuracy is unknown.

Interpreting our calculation one should keep in mind the following restriction. Since the MC data for large $r$ are not available, we cannot say how the Hubbard-I approximation fares for $r$ exceeding 5–6 lattice constants. The MC data of [10] cannot be used to rule out the possibility that the Hubbard model exhibits superconductivity with the correlation length larger than 5–6 lattice constants. Our method in its present form is too crude to capture the superconducting correlations.

To conclude, generalizing the Hubbard-I approximation we derive the equation of motion for the two-particle propagator. For the square lattice of finite size this equation is solved numerically. It is demonstrated that the Hubbard-I propagator is consistent with the MC data up to a numerical coefficient of order 3. Thus, the Hubbard-I method can be used to approximate the two-particle propagator of the Hubbard model, at least at a qualitative level and at moderate separations.

**Acknowledgments**

The authors would like to thank Professor Imada who kindly provided the Monte Carlo data shown in figures 1 and 2. Discussions with M Yu Kagan are gratefully acknowledged. The support of RFBR (grants 09-02-00248, 09-02-92114, 08-02-00212) is also acknowledged.

**Appendix A. Derivation of equation (19)**

Here we obtain equation (19) assuming that $i \neq j$ and $i \neq m$.

The equation of motion for $\tilde{P}_{\text{lm}}$ is

$$\tilde{P}_{\text{lm}} = \langle \tilde{T}C(\tau) \Delta_{\text{lm}}(0) \rangle + \delta(\tau) \{ (n_{\bar{i} \bar{j}} + n_{\bar{j} \bar{i}}) \Delta_{\bar{i} \bar{j}} \},$$

(A.1)

where we introduced the notation

$$C = [H, (n_{\bar{i} \bar{j}} + n_{\bar{j} \bar{i}}) \Delta_{\bar{i} \bar{j}}]$$

$$= [(H_{\text{kin}} + H_{\text{int}}), (n_{\bar{i} \bar{j}} + n_{\bar{j} \bar{i}}) \Delta_{\bar{i} \bar{j}}] - 2\mu (n_{\bar{i} \bar{j}} + n_{\bar{j} \bar{i}}) \Delta_{\bar{i} \bar{j}}.$$  

(A.2)

Neglecting ‘double-occupancy’ terms in the commutator with $H_{\text{kin}}$, we get

$$[H_{\text{kin}}, (n_{\bar{i} \bar{j}} + n_{\bar{j} \bar{i}}) \Delta_{\bar{i} \bar{j}}] \approx -i \sum_a n_{\bar{i} \bar{j}} c_{\bar{i} \bar{j}}^+ c_{\bar{i} \bar{j}} \langle 1 - \delta_{\bar{i} \bar{j} + a} \rangle$$

$$+ n_{\bar{j} \bar{i}} c_{\bar{j} \bar{i}}^+ c_{\bar{j} \bar{i}} \langle 1 - \delta_{\bar{i} \bar{j} + a} \rangle$$

$$+ n_{\bar{i} \bar{j}} c_{\bar{i} \bar{j}}^+ c_{\bar{i} \bar{j}} \langle 1 - \delta_{\bar{i} \bar{j} + a} \rangle$$

$$+ n_{\bar{j} \bar{i}} c_{\bar{j} \bar{i}}^+ c_{\bar{j} \bar{i}} \langle 1 - \delta_{\bar{i} \bar{j} + a} \rangle.$$  

(A.3)

The factors of the type $1 - \delta_{\bar{i} \bar{j}}$ appear for the following reason. Consider

$$n_{\bar{i} \bar{j}} c_{\bar{i} \bar{j}}^+ c_{\bar{i} \bar{j}} = n_{\bar{j} \bar{i}} c_{\bar{i} \bar{j}}^+ c_{\bar{i} \bar{j}} \langle 1 - \delta_{\bar{i} \bar{j} + a} \rangle - n_{\bar{i} \bar{j}} c_{\bar{i} \bar{j}}^+ c_{\bar{i} \bar{j}} \delta_{\bar{i} \bar{j} + a}. $$  

(A.4)
The last term corresponds to the case of two electrons at the same site, \( i = j \neq \alpha \). It is small and can be omitted. Applying the Hubbard-I decoupling and taking into account that in the absence of the magnetization \( \langle c_{\alpha \beta}^+ c_{\alpha \beta}^- \rangle = 0 \), we obtain

\[
H_{\text{kin}}. (n_{i\beta} + n_{j\sigma}) \Delta_{ij} \approx -t \sum_{\alpha} \langle n_{i\alpha}\rangle c_{i\alpha \sigma}^+ c_{j\beta}^- (1 - \delta_{i+a}) + \langle n_{i\gamma}\rangle c_{i\gamma \sigma}^+ c_{j\beta}^- (1 - \delta_{i+a}).
\]

Then, we calculate the commutator with \( H_{\text{int}} \):

\[
[H_{\text{int}}. (n_{i\beta} + n_{j\sigma}) \Delta_{ij}] = (n_{i\sigma} + n_{j\alpha}) \left[ H_{\text{int}}, \Delta_{ij} \right] = U(n_{i\beta} + n_{j\gamma})^2 \Delta_{ij}.
\]

We note that \( n_{i\beta}^2 = n_{j\sigma} \) and \( U(n_{i\beta} + n_{j\gamma}) \Delta_{ij} = O(t/U) \). As a result, it holds that

\[
[H_{\text{int}}. (n_{i\beta} + n_{j\sigma}) \Delta_{ij}] \approx U(n_{i\beta} + n_{j\gamma}) \Delta_{ij}.
\]

Collecting all the terms together, we derive

\[
[H_{\text{int}}. (n_{i\beta} + n_{j\sigma}) \Delta_{ij}] \approx -t(n_{i\sigma}) \sum_{\alpha} c_{i\alpha \sigma}^+ c_{j\beta}^- (1 - \delta_{i+a}) + c_{i\alpha \sigma}^+ c_{j\beta}^- (1 - \delta_{i+a}) + U(n_{i\beta} + n_{j\gamma}) \Delta_{ij},
\]

where we define \( \langle n_{i\sigma} \rangle = \langle n_{j\beta} \rangle = \langle n_{j\alpha} \rangle \). Finally, we calculate the commutator:

\[
[H_{\text{int}}, (n_{i\beta} + n_{j\sigma}) \Delta_{ij}] \approx \langle n_{i\beta} \rangle c_{i\gamma \sigma}^+ c_{j\gamma}^- \delta_{ij} - \langle n_{i\gamma} \rangle c_{i\alpha \sigma}^+ c_{j\alpha}^- \delta_{ij},
\]

Obtaining this result, we took into account that in the absence of the magnetic order,

\[
\langle c_{i\alpha \sigma}^+ c_{j\gamma}^- \rangle = \langle c_{i\gamma \sigma}^+ c_{j\alpha}^- \rangle = 0.
\]

Further, in (A.10) the terms

\[
n_{i\beta} c_{i\gamma \sigma}^+ c_{j\alpha}^- \delta_{ij} = O(t/U) \quad \text{ and } \quad c_{i\alpha \sigma}^+ n_{j\gamma} c_{j\alpha}^- = O(t/U)
\]

are dropped. Besides, we performed Hubbard-I decoupling in three-site operators:

\[
n_{j\sigma} c_{i\alpha \beta} c_{k\gamma} \approx \langle n_{j\sigma} \rangle c_{i\alpha \beta} c_{k\gamma} (1 - \delta_{i\gamma}) \quad \text{and} \quad c_{i\alpha \sigma}^+ n_{j\gamma} c_{j\beta}^+ \approx O(t/U).
\]

In (A.13) we used the fact that \( n_{j\beta} c_{i\gamma \sigma} \delta_{ij} = 0 \). As a result, within the scope of our approximation, (A.1) can be written as

\[
\hat{P}_{\text{lim}} \approx -t(n_{i\sigma}) \sum_{\alpha} \left[ P_{i\sigma \alpha} \delta_{ij} + P_{i\sigma \alpha \sigma} (1 - \delta_{i+a}) \right] + (U-2\mu) \hat{P}_{\text{lim}+} + \delta(\tau)(n_{i\sigma})(c_{i\alpha \sigma}^+ c_{j\beta}^- - c_{i\alpha \sigma}^- c_{j\beta}^+ - \delta_{ij}).
\]

Since \( P = O(t/U) \) while \( P = O(1) \), we omit \( \hat{P} \) and \( \mu \hat{P} \) terms, arriving at (19).

### Appendix B. Fourier transformation

To solve (21), analytically or numerically, it is useful to subject this equation to the Fourier transformation. Let us consider a square 2D lattice with the number of sites \( N = M \times M \). In Fourier space, (21) reads

\[
P_{k,i;k',k';\omega} = \frac{1}{N^2} \sum_{\alpha} \left( c_{k\alpha \sigma}^+ e^{ik\cdot n_c} + c_{k\alpha \sigma} \right) = S + R.
\]

Here

\[
S = \frac{1}{N^2} \sum_{\alpha} \left( c_{k\alpha \sigma}^+ + c_{k\alpha \sigma} \right) P_{i\sigma \alpha} \delta_{ij} + \delta_{ij}(k_{\alpha \sigma}) \delta_{k_{\alpha \sigma}},
\]

\[
R = \frac{1}{N^2} \sum_{\alpha} \left( c_{k\alpha \sigma}^+ - c_{k\alpha \sigma} \right) \delta_{k_{\alpha \sigma}},
\]

After straightforward algebra we derive

\[
S = \frac{\delta_{ij}}{N} \sum_{\alpha} \left( \gamma_{k_{\alpha}} + \gamma_{k_{\alpha}} - \gamma_{k_{\alpha}} + \gamma_{k_{\alpha}} \right) P_{i\sigma \alpha} \delta_{ij} + \delta_{ij}(k_{\alpha \sigma}),
\]

where the number of nearest neighbours in the lattice, \( z \), is 4, and we introduce the notation

\[
\gamma_{k_{\alpha}} = \frac{1}{z} \sum_{\alpha} \exp(ika).
\]

The term \( R \) in the right-hand side of (B.1) is transformed with the help of the formula for the single-electron Green’s function in the Hubbard-I approximation:

\[
\langle c_{k\alpha \sigma}^+ c_{k\alpha \sigma} \rangle = -(1 - \langle n_{i\sigma} \rangle) G_0(i - j, +0),
\]

where \( G_0 \) is the Green’s function for free fermions. From this equation it follows that

\[
\langle c_{k\alpha \sigma}^+ c_{k\alpha \sigma} \rangle = \frac{1}{1 - \langle n_{i\sigma} \rangle} [1 - \gamma_{k_{\alpha}}(\delta_{k_{\alpha}} - \mu)],
\]

where \( n_F \) is the Fermi distribution function, and \( \delta_{k_{\alpha}} \) is the energy spectrum. In the case of the square lattice and strong electron-electron repulsion \( U \gg zt \) considered, we can write in the tight-binding approximation \( \delta_{k_{\alpha}} = zt \gamma_{k_{\alpha}} \).

Within the Hubbard-I approach the expectation value \( \langle c_{k\alpha \sigma}^+ c_{k\alpha \sigma} \rangle \) satisfies

\[
\langle c_{k\alpha \sigma}^+ c_{k\alpha \sigma} \rangle = -(1 - \langle n_{i\sigma} \rangle) (1 + \langle n_{i\sigma} \rangle) \delta_{ij}.
\]

This expression is incompatible with the usual Fermi anticommutation rules. This is an artefact of the Hubbard-I scheme, a discrepancy which is a consequence of the inexact nature of the Hubbard-I Green’s functions. This means that the Hubbard-I Green’s function fails at energy higher than \( \tilde{t} \), or, equivalently, at \( |i - j| \) smaller than at least several lattice constants.

Using the above relations we derive, after simple algebra,

\[
R = \frac{1}{M^2} \left[ n_F(\delta_{k_{\alpha}} - \mu) + n_F(\delta_{k_{\alpha}} - \mu) - 1 \right] \delta_{k_{\alpha}} \delta_{k_{\alpha}}.
\]
Combining the expressions for $S$ and $R$, we can rewrite (B.1) in the form

$$\begin{align*}
\left[ i\omega + z\bar{f}(\gamma_{k_1} + \gamma_{k_2}) + 2\mu \right] P_{k_1 k_2; k_3 k_4} = & \frac{z\bar{f}}{M} \sum_{q} \left( \gamma_{k_1 + q, k_2 - q} + \gamma_{k_2 + q, k_1 - q} \right) P_{k_1 - q, k_2 + q; k_3 k_4} \\
& + \left( 1 - (n_{\sigma})^2 \right) \left[ n_F(\delta_{k_3}, -\mu) + n_F(\delta_{k_4}, -\mu) - 1 \right] \delta_{k_3 k_4}.
\end{align*}$$

(B.8)

The propagator $P_{k_1 k_2; k_3 k_4}$ is non-zero only if $k_1 + k_2 = k_3 + k_4$. This is a consequence of the momentum conservation law.

Therefore, it is convenient to introduce the total momentum $k_1 + k_2 = Q$ and define

$$P_{Q; k_3 k_4} = P_{k_1 k_2; Q}.$$ 

(B.9)

Equation (B.8) can be rewritten as

$$\begin{align*}
i \omega P_{Q; k_3 k_4} = & \sum_{q} I_{Q}^{Q}_{k_3 k_4} P_{Q; k_3 k_4} + \mathcal{R}_{Q}^{Q}_{k_3 k_4},
\end{align*}$$

(B.10)

where

$$I_{Q}^{Q}_{k_3 k_4} = -\frac{z\bar{f}}{M} \sum_{q} \left( \gamma_{Q - k_3, Q - k_4} + 2\mu \right) \delta_{k_3 k_4},$$

$$\mathcal{R}_{Q}^{Q}_{k_3 k_4} = \left( 1 - (n_{\sigma})^2 \right) \frac{z\bar{f}}{M^2} \sum_{q} \left[ n_F(\delta_{Q - k_3, -\mu}) + n_F(\delta_{Q - k_4, -\mu}) - 1 \right] \delta_{k_3 k_4}.$$ 

(B.11)

(B.12)

and (B.10) may be used to calculate the propagator $P$.

Appendix C. Computation of the equal-time correlation function

Equation (B.10) may be cast in the matrix form $i \omega P = hP + \mathcal{R}$. Matrix $h$ is symmetric and, consequently, can be diagonalized.

We write down $h$ symbolically as $h = U d U^T$, where $d$ is a diagonal matrix with the diagonal elements $d_i$:

$$d = \text{diag}(d_i).$$

(C.1)

$U$ is a unitary matrix, and $U^T$ is its Hermitian-conjugate matrix. Thus, the solution of the problem can be expressed in the form

$$P(\omega) = \left( U(i\omega - d) U^T \right)^{-1} \mathcal{R}.$$ 

(C.2)

We diagonalize the matrix $h$ numerically and calculate the equal-time propagator $P_{\pm \infty}(+0) = (\Delta_{\pm} \Delta_{\pm})$, performing frequency summation:

$$P(\tau \to +0) = T \sum_{\omega} \exp(i\tau \omega) P(\omega) \bigg|_{\tau \to +0}$$

(C.3)

according to the rule

$$\begin{align*}
T \sum_{\omega} \exp(i\tau \omega) (\omega - \mu)^{-1} \bigg|_{\tau \to +0} = N_B(d),
\end{align*}$$

where $N_B(\epsilon) = (e^{\epsilon/T} - 1)^{-1} \text{ is the Bose distribution function, and } N_B(d) \text{ is a diagonal matrix: } N_B(d) = \text{diag}[N_B(d_i)].$ As a result, we derive

$$P(\tau \to 0) = U N_B(d) U^T \mathcal{R}.$$ 

(C.4)

This equation can be used to calculate the correlation function numerically.

References

[1] Hubbard J 1963 Proc. R. Soc. A 276 238
[2] Kohn W and Luttinger J M 1965 Phys. Rev. Lett. 15 524
[3] Scalapino D J, Koh E J and Hirsch J E 1986 Phys. Rev. B 34 8190
[4] Koikegami S and Yanagisawa T 2006 J. Phys. Soc. Japan 75 034715
[5] Yanagisawa T 2008 New J. Phys. 10 023014
[6] Baranov M A and Kagan M Yu 1992 Z. Phys. B 86 237
[7] Baranov M A, Chubukov A V and Kagan M Yu 1992 Int. J. Mod. Phys. B 6 2471
[8] Kagan M Yu, Fresard R, Capezzali M and Beck H 1998 Phys. Rev. B 57 5995
[9] Zhang S, Carlson J and Gubernatis J E 1997 Phys. Rev. Lett. 78 4486
[10] Aimi T and Imada M 2007 J. Phys. Soc. Japan 76 113708
[11] Yokoyama H, Tanaka Y, Ogata M and Tsuchiura H 2004 J. Phys. Soc. Japan 73 1119
[12] Maier T A, Jarrell M, Schulthess T C, Kent P R C and White J B 2005 Phys. Rev. Lett. 95 237001
[13] Sénéchal D, Lavertu P-L, Marois M-A and Tremblay A-M S 2005 Phys. Rev. Lett. 94 156404
[14] Capone M and Kotliar G 2006 Phys. Rev. B 74 054513
[15] Aichhorn M, Arrigoni E, Potthoff M and Hanke W 2006 Phys. Rev. B 74 024508
[16] Yokoyama H, Ogata M and Tanaka Y 2006 J. Phys. Soc. Japan 75 114706
[17] Baeriswyl D, Eichenberger D and Menteshashvili M 2009 New J. Phys. 11 075010
[18] Homecki T and Wosiek L 1999 J. Phys. B 32 09173
[19] Mierzejewski M 1996 J. Supercond. 9 293
[20] Zielinski J, Mierzejewski M and Entel P 1998 Phys. Rev. B 57 10331
[21] Mierzejewski M, Zielinski J and Entel P 1998 Acta Phys. Pol. B 29 3907
[22] Cebula A and Zielinski J 1999 J. Supercond. 12 649
[23] Caixão E S and Troper A 2008 Physica B 403 1071
[24] Caixão E S and Troper A 2008 J. Magn. Magn. Mater. 320 490
[25] Been J and Edwards D M 1995 Phys. Rev. B 52 13636
[26] Calegari E J, Magalhães S G and Gomes A A 2005 Eur. Phys. J. B 45 485
[27] Plakida N M 1998 Condens. Matter Phys. 1 57
[28] Ovchinnikov S G and Val’kov V V 2004 Hubbard Operators in the Theory of Strongly Correlated Electron (London: Imperial College Press)
[29] Zaitsev R O 2007 Diagrammatic Methods in the Theory of Superconductivity and Ferromagnetism (Moscow: URSS)
[30] Corney J F and Drummond P D 2006 Phys. Rev. B 73 125112
[31] Corney J F and Drummond P D 2006 J. Phys. A: Math. Gen. 39 269
[32] Aimi T and Imada M 2007 J. Phys. Soc. Japan 76 084709