Comparison of Variational Approaches for the Exactly Solvable
1/r-Hubbard Chain

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Abstract

We study Hartree-Fock, Gutzwiller, Baeriswyl, and combined Gutzwiller-Baeriswyl wave functions for the exactly solvable one-dimensional 1/r-Hubbard model. We find that none of these variational wave functions is able to correctly reproduce the physics of the metal-to-insulator transition which occurs in the model for half-filled bands when the interaction strength equals the bandwidth. The many-particle problem to calculate the variational ground state energy for the Baeriswyl and combined Gutzwiller-Baeriswyl wave function is exactly solved for the 1/r-Hubbard model. The latter wave function becomes exact both for small and large interaction strength, but it incorrectly predicts the metal-to-insulator transition to happen at infinitely strong interactions. We conclude that neither Hartree-Fock nor Jastrow-type wave functions yield reliable predictions on zero temperature phase transitions in low-dimensional, i.e., charge-spin separated systems.

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I. INTRODUCTION

Variational wave functions are often used to study ground state properties of quantum mechanical many-particle systems. Examples of approximate ground state wave functions for correlated Fermions are Hartree-Fock [1], Gutzwiller [2], local Ansatz [3], and, in general, Jastrow-Feenberg wave functions [4]. One of the advantages of variational wave functions is the fact that they give an exact upper bound for the true ground state energy. Thus there is, at least in principle, a criterion to assess variational wave functions: the lower the variational ground state energy, i.e., the tighter the variational bound, the better the wave function (“energy criterion”).

In practice, however, two major problems arise: (i) the energy might not be a good criterion for the “quality” of a wave function, i.e., a wave function might give a very good approximation for the ground state energy but it may still miss the ground state physics of the system under consideration. This issue can, however, only be addressed, if the exact solution of the corresponding Hamiltonian is known; (ii) the evaluation of correlated wave functions poses yet another quantum many-particle problem such that even seemingly simple wave functions (and their straightforward improvements) are not analytically tractable.

To deal with these two problems we focus on the exactly solvable one-dimensional $1/r$-Hubbard model [5]. It describes spin-1/2 Fermions on a chain of $L$ sites, hopping with long-range amplitude, $t_{l,m} = it(-1)^{l-m} [d(l-m)]^{-1} = t_{m,l}^*$. Here, $d(l-m) = (L/\pi) \sin[\pi(l-m)/L]$ is the chord distance between sites $l$ and $m$ on the chain closed into a ring (the lattice spacing $a$ is set to unity). The hopping becomes $t_{l,m} \rightarrow it/(l-m)$ in the thermodynamical limit $L \rightarrow \infty$ for fixed distance $(l-m)$ (“1/r-hopping”). The electrons interact through a local Hubbard [6] interaction, $U$, and the total 1/r-Hubbard Hamiltonian reads

$$\hat{H} = \hat{T} + U \hat{D} = \sum_{l \neq m=1,\sigma}^{L} t_{l,m} \hat{c}_{l,\sigma}^{\dagger} \hat{c}_{m,\sigma} + U \sum_{l=1}^{L} \hat{n}_{l,\uparrow} \hat{n}_{l,\downarrow}. \tag{1}$$

For even $L$ we choose antiperiodic boundary conditions, so that the resulting dispersion relation is linear in wave vector, namely, $\epsilon(k) = tk$ with $k = \Delta(m + 1/2)$ ($\Delta = 2\pi/L$, ...
\( m = -L/2, \ldots, L/2 - 1 \). For \( U = 0 \) the Fermi sea is the ground state with all \( k \)-states from \( k = -\pi \) to \( k_F = \pi(n-1) \) filled where \( n = (N_\uparrow + N_\downarrow)/L \) is the total particle density. For half-filling \( (n = 1) \) and \( U \to \infty \), the Hamiltonian \( (\mathbb{I}) \) reduces to the spin-1/2 \((1/r)^2\)-Heisenberg or Haldane-Shastry model \( (\mathbb{H}) \). In the rest of the paper we will restrict ourselves to \( n \leq 1 \). The more than half-filled case can be obtained by particle-hole symmetry \( (\mathbb{S}) \).

The exact solution of the \( 1/r \)-Hubbard Hamiltonian was conjectured in Ref. \( (\mathbb{R}) \), and its physical properties were discussed in detail elsewhere \( (\mathbb{S}) \). The model displays a Mott-Hubbard metal-to-insulator transition at half-filling when the interaction strength, \( U \), equals the bandwidth, \( W = 2\pi t \). This is in contrast to the one-dimensional Hubbard model which was exactly solved by Lieb and Wu \( (\mathbb{E}) \). There, the tight-binding cosine dispersion has a perfect nesting wave vector \( q = \pi \) such that \( \epsilon_{tb}(k) = -2t \cos k = -\epsilon_{tb}(k + q) \). Consequently, the Hubbard model describes an insulating state for all \( U > 0 \) at half-filling. This metal-to-insulator transition at \( U = 0^+ \) for \( n = 1 \) is trivially reproduced in an antiferromagnetic Hartree-Fock theory \( (\mathbb{F}) \). We therefore use the \( 1/r \)-Hubbard model to assess the quality of the Hartree-Fock approach for models without the perfect nesting property.

Another advantage of the \( 1/r \)-Hubbard model comes from the fact that we are able to calculate variational ground state energies for correlated wave functions without further approximations. Thus far, this was only achieved for the Gutzwiller wave function in one dimension \( (\mathbb{G}, \mathbb{I}) \), or, for general Gutzwiller-correlated wave functions, in the limit of large dimensions \( (\mathbb{J}, \mathbb{L}) \) or large orbital degeneracies \( (\mathbb{M}) \). For the \( 1/r \)-Hubbard model we are able to derive the ground state energies for the Baeriswyl \( (\mathbb{F}) \) and a combined Gutzwiller-Baeswyl wave function.

The plan of the paper is as follows: in section \( (\mathbb{P}) \) we diagonalize the antiferromagnetic Hartree-Fock Hamiltonian to obtain the Hartree-Fock ground state wave function and energy. In section \( (\mathbb{Q}) \) we introduce and evaluate the Gutzwiller-, Baeriswyl-, and Gutzwiller-Baeswyl wave functions. We draw our conclusions on the quality of these variational approaches in section \( (\mathbb{V}) \).
II. HARTREE FOCK APPROXIMATION

As usual we factorize the interaction part of the Hamiltonian as

\[ \hat{n}_{l,\uparrow} \hat{n}_{l,\downarrow} \rightarrow \langle \hat{n}_{l,\uparrow} \rangle \langle \hat{n}_{l,\downarrow} \rangle + \langle \hat{n}_{l,\uparrow} \rangle \langle \hat{n}_{l,\downarrow} \rangle - \langle \hat{n}_{l,\uparrow} \rangle \langle \hat{n}_{l,\downarrow} \rangle \] (2a)

and allow for a sublattice magnetization

\[ m = |\langle \hat{n}_{l,\uparrow} \rangle - \langle \hat{n}_{l,\downarrow} \rangle| \]

alternating in sign on the odd/even lattice points of the A-B lattice. The particle density

\[ n = \langle \hat{n}_{l,\uparrow} \rangle + \langle \hat{n}_{l,\downarrow} \rangle \]

remains uniform. Thus we may write

\[ \langle \hat{n}_{l,\sigma} \rangle = \frac{n}{2} + (-1)^l \sigma \frac{m}{2} . \] (2b)

We introduce the new quasiparticle operators \( \hat{a}_{k,\sigma}, \hat{b}_{k,\sigma} \) within the magnetic Brillouin zone \(-\pi < k < 0\) by

\[
\begin{align*}
\hat{a}_{k,\sigma} &= \cos \phi_{k,\sigma} \hat{c}_{k,\sigma} + \sin \phi_{k,\sigma} \hat{c}_{k+\pi,\sigma} \\
\hat{b}_{k,\sigma} &= -\sin \phi_{k,\sigma} \hat{c}_{k,\sigma} + \cos \phi_{k,\sigma} \hat{c}_{k+\pi,\sigma}
\end{align*}
\] (3a)

and the inverse transformation reads

\[
\begin{align*}
\hat{c}_{k,\sigma} &= \cos \phi_{k,\sigma} \hat{a}_{k,\sigma} - \sin \phi_{k,\sigma} \hat{b}_{k,\sigma} \\
\hat{c}_{k+\pi,\sigma} &= \sin \phi_{k,\sigma} \hat{a}_{k,\sigma} + \cos \phi_{k,\sigma} \hat{b}_{k,\sigma}
\end{align*}
\] (3b)

The band width of our model is \( W = 2\pi t \), and the transformation angle \( \phi_{k,\sigma} \) fulfills

\[
\begin{align*}
\tan 2\phi_{k,\sigma} &= \sigma \frac{2Um}{W} \\
\sin^2 \phi_{k,\sigma} &= \frac{1}{2} \left( 1 - \sigma \frac{W}{\sqrt{W^2 + (2Um)^2}} \right)
\end{align*}
\] (4a)

The operators are constructed such that \( \hat{a}_{k,\sigma}^+ (\hat{b}_{k,\sigma}^+) \) creates particles mainly on the A-lattice (B-lattice) sites. The Hartree-Fock Hamiltonian then reads

\[
\hat{H}_{HF} = \sum_{-\pi < k < 0} E_k^- \left( \hat{a}_{k,\downarrow}^+ \hat{a}_{k,\downarrow} + \hat{b}_{k,\downarrow}^+ \hat{b}_{k,\downarrow} \right) + E_k^+ \left( \hat{a}_{k,\uparrow}^+ \hat{a}_{k,\uparrow} + \hat{b}_{k,\uparrow}^+ \hat{b}_{k,\uparrow} \right)
\] (5a)

with
The Hartree-Fock charge gap is given by
\[ \Delta \mu_{HF}^+ = E_{k=-\pi}^+ - E_{k=0}^- = \left[ \sqrt{W^2 + 4U^2m^2} - W \right]/2. \]

The corresponding ground state wave function reads
\[ |\psi_0^{\text{HF}}\rangle = \prod_{-\pi<k<k^{HF}} \hat{a}_{k,\uparrow}^+ \hat{b}_{k,\downarrow}^+ |\text{vacuum}\rangle. \]

Finally, we obtain the particle densities for all temperatures \( T = 1/\beta \) as
\[ \langle \hat{n}_{k,\uparrow}^a \rangle = \frac{1}{\exp \left( \beta(E_k^--\mu_{HF}) \right) + 1} = f_{\text{FD}}(E_k^-) = \langle \hat{n}_{k,\downarrow}^b \rangle \] (7a)
\[ \langle \hat{n}_{k,\uparrow}^b \rangle = \frac{1}{\exp \left( \beta(E_k^+-\mu_{HF}) \right) + 1} = f_{\text{FD}}(E_k^+) = \langle \hat{n}_{k,\downarrow}^a \rangle \] (7b)

where the Hartree-Fock chemical potential \( \mu_{HF} \) is obtained from the particle number
\[ n = \frac{1}{L} \sum_{-\pi<k<\pi,\sigma} \langle \hat{n}_{k,\sigma} \rangle = \frac{2}{2\pi} \int_{-\pi}^{\pi} dk \left[ f_{\text{FD}}(E_k^-) + f_{\text{FD}}(E_k^+) \right]. \] (8a)

The self-consistency condition reads
\[ m = |\langle \hat{n}_{\uparrow} \rangle - \langle \hat{n}_{\downarrow} \rangle| \]
\[ = \frac{4Um}{\sqrt{W^2 + 4U^2m^2}} \left| \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \left[ f_{\text{FD}}(E_k^-) - f_{\text{FD}}(E_k^+) \right] \right|. \] (8b)

This equation gives the magnetization as a function of temperature and interaction strength.

We note that the Hartree-Fock Hamiltonian (5a) will give a finite magnetization at finite temperatures, if \( m > 0 \) at \( T = 0 \). However, a phase transition from a paramagnetic to an antiferromagnetic phase at some finite Neél temperature does not happen in a one-dimensional system \([18]\). This is one of the well-known shortcomings of the Hartree-Fock Mean-Field approach to low-dimensional systems. Furthermore, it gives a \( T = 0 \) transition to a magnetic phase at a critical value \( U = U_{HF}^c(n) \) for all band-fillings because a finite magnetization is the only way to obtain a lower energy than the paramagnetic Hartree-Fock phase for large \( U/W \). We thus restrict ourselves to the half-filled case \((n = 1)\) where the Hartree-Fock approach gives the best results. For \( n < 1 \) the antiferromagnetic Hartree-Fock theory certainly fails to give the correct physical picture.
In the case of half-filling the Hartree-Fock chemical potential follows from eq. (8a) to be temperature independent. It is given by \( \mu_{\text{HF}} = U (1 + m^2) / 4 \) which lies in the middle of the gap between the upper and lower Hartree-Fock band. The self-consistency equation (8b) for the magnetization does not considerably simplify but stays an implicit equation which has to be solved numerically for \( T > 0 \). Here, we are only interested in ground state properties. For \( \beta \to \infty \) the lower Hartree-Fock band is completely filled (\( k_{\text{HF}}^F = 0 \)), and it follows from (8b) that either \( m = 0 \) (paramagnetic Hartree-Fock solution) or

\[
2U = \sqrt{W^2 + 4U^2m^2}.
\]

Hence, Hartree-Fock predicts a transition from a paramagnetic metal to an antiferromagnetic insulator at \( U_{c}^{\text{HF}}(n = 1) = W/2 \), above which we have \( m = \sqrt{1 - (U_{c}^{\text{HF}}/U)^2} \) with the typical mean-field exponent of one-half near the transition. The charge gap is \( \Delta \mu_{c}^{\text{HF}} = (\sqrt{W^2 + 4U^2m^2} - W) / 2 = U - U_{c}^{\text{HF}} \). The Hartree-Fock gap grows linearly as a function of \( U - U_{c}^{\text{HF}} \) in agreement with the exact solution \([3,8]\) where, however, the true transition is at twice the Hartree-Fock value, \( U_{c} = 2U_{c}^{\text{HF}} \). It is amusing to note that the density of states for spinon excitations develops a van-Hove singularity (formation of the upper and lower Hubbard band) precisely at \( U = W/2 \) \([8]\). It is again seen that antiferromagnetic Hartree-Fock is sensitive to spin-correlations only.

The Hartree-Fock variational ground state energy density at half-filling is given by \( e_{0}^{\text{HF}} = (1/L) \sum_{\pi,\pi<k<0} E_k \) which gives

\[
e_{0}^{\text{HF}} = \begin{cases} 
\frac{U - W}{4} & \text{for } U \leq W/2 \ (m = 0) \\
-\frac{W^2}{16U} & \text{for } U \geq W/2 \ (m = \sqrt{1 - (W/2U)^2})
\end{cases}
\]

which is compared in fig. 1 to the exact ground state energy

\[
e_0 = \begin{cases} 
\frac{U - W}{4} - \frac{U^2}{12W} & \text{for } U \leq W \\
-\frac{W^2}{12U} & \text{for } U \geq W
\end{cases}.
\]

It is seen that Hartree-Fock, as an effective single-particle theory, fails to give any contribution to the correlation energy of order \( U^2/W \). There are no non-analytic contributions
of the order \(\exp(-W/U)\) for small \(U/W\) as expected for a Hamiltonian without the perfect nesting property.

At large \(U/W\) it gives the correct analytical behavior with a smaller prefactor. However, it also predicts a finite sublattice magnetization which is, of course, zero in the exact solution. Furthermore, the Hartree-Fock gap is temperature dependent and one gets a transition from an antiferromagnetic insulator to a paramagnetic metal as function of temperature, if \(U > U_{\text{c}}^{\text{HF}}\). The gap in the exact solution is temperature independent, and no transitions occur at finite \(T\). Finally, the zero temperature transition itself in Hartree-Fock is driven by spin-correlations. This can be seen from the fact that one has a finite sublattice magnetization after the transition, and that the transition happens at all fillings. This is in contrast to the exact solution where the transition happens only at half-filling, and no magnetic ordering occurs. Hence, the transition in the 1/r-Hubbard model is driven by charge-correlations, just opposite to the physics of the Hartree-Fock approximation.

### III. CORRELATED WAVE FUNCTIONS

We now focus on the correlated wave functions whose energy we want to evaluate. Our starting point is the Gutzwiller wave function [4]

\[
|\psi_G(g)\rangle = g^D |\text{Fermi-sea}\rangle = \prod_{l=1}^{L} \left[1 - (1 - g) \hat{D}_l\right] |\text{Fermi-sea}\rangle
\]  

which starts from the Fermi-sea, the exact ground state for \(U = 0\) (\(g = 1\)). For \(U > 0\) double occupancies are less favorite because of the on-site repulsion in the Hamiltonian, eq. (1). To include this effect, double occupancies are suppressed by the Gutzwiller correlator \(\prod_{l=1}^{L} \left[1 - (1 - g) \hat{D}_l\right]\) which globally reduces configurations with double occupancies in the Fermi-sea, if \(g < 1\). Note that this correlator is regular for all \(0 < g < 1\), i.e., \(|\psi_G(g)\rangle\) describes a (correlated) metal as long as we do not project out all double occupancies. For \(g = 0\) we alter the nature of the Fermi-sea because we not only suppress configurations with double occupancies but truly eliminate them with the help of the Gutzwiller projector \(\hat{P}_{D=0} = \prod_{l=1}^{L} \left[1 - \hat{D}_l\right]\).
A metal-to-insulator transition within this wave function can only be expected at half-filling, if the variational procedure gives $g = 0$ such that every site is singly occupied (for less than half-filling the remaining holes are still mobile and keep the state metallic). Brinkman and Rice observed that such a transition ("Brinkman-Rice transition" [19,20]) at a finite $U = U_c^{BR} = 8|\epsilon_0^{FS}|$ was contained in the Gutzwiller Approximation [2] to the Gutzwiller wave function, where $\epsilon_0^{FS}$ is the kinetic energy of the Fermi-sea in the non-interacting system. It was later understood that this approximation becomes exact in the limit of infinite dimensions [10,13]. If we plainly apply the Gutzwiller Approximation to our one-dimensional system we obtain $\epsilon_0^{FS} = -W/4$, $U_c^{BR} = 2W$, and the ground state energy density at half-filling in the Gutzwiller Approximation is given by $\epsilon_0^{GA} = \epsilon_0^{FS}(1 - U/U_c^{BR})^2$ for $U \leq U_c^{BR}$, $\epsilon_0^{GA} = 0$ for $U \geq U_c^{BR}$. This energy density is plotted in figure 1 in comparison to the Hartree-Fock and the exact result. Although the Gutzwiller Approximation is an uncontrolled approximation in any finite dimension, we obtain the interesting result that it predicts a metal-to-insulator transition at half-filling for a finite value $U = U_c^{BR} = 2W$. This transition is driven by charge-correlations only which is obvious from the fact that the ground state energy density in this approximation is zero beyond $U_c^{BR}$. It is thus seen that this approximation very accurately describes the physical mechanism of the metal-to-insulator transition in our one-dimensional model, despite the fact that it is not variationally controlled, and the variational estimate for the ground state energy density is poor for large $U/W$. In any finite dimension, the Brinkman-Rice transition will be shifted to $U_c^G = \infty$ where double occupancies are strictly forbidden by the Hubbard interaction. This has indeed been proven for the Gutzwiller wave function [21].

It was only recently that one was able to go beyond the Gutzwiller Approximation to exactly evaluate the Gutzwiller wave function in one dimension [14,11]. It was shown that the Gutzwiller wave function does not give a good ground state energy for the one-dimensional Hubbard model for large $U/W$ due to poor correlations between double occupancies and holes [12]. On the other hand, the correlations between spins are excellent such that the Gutzwiller projected Fermi-sea is a very good trial state for the one-dimensional antiferro-
magnetic Heisenberg model \[22,11,12\]. We will see below that these considerations remain valid for the $1/r$-Hubbard model, eq. (1).

Baeriswyl \[17\] constructed a variational wave function for the one-dimensional Hubbard model to overcome the difficulties of the Gutzwiller wave function for large $U/W$. He started from the Gutzwiller-projected Fermi-sea to incorporate its excellent spin correlations, and proposed

$$|\psi_B(b)\rangle = b^{\hat{T}/W} \hat{P}_{D=0}|\text{Fermi-sea}\rangle$$

(13)
as variational ground state ($0 \leq b \leq 1$). For large $U/W$ the variational parameter $b$ is close to unity, and double occupancies and holes are linked by the application of the kinetic energy operator to the Gutzwiller-projected Fermi-sea. Hence, the missing charge-correlations in the Gutzwiller wave function are now properly taken into account \[17\].

At half-filling, the Baeriswyl wave function describes an insulator for all $0 < b \leq 1$ because the Gutzwiller-projected half-filled Fermi-sea is insulating, and the Baeriswyl-correlator $b^{\hat{T}/W}$ is regular as long as $b > 0$. A metal-to-insulator transition will only happen, if $b = 0$ is the result of the minimization procedure. Since $b = 0$ corresponds to the free Fermi-sea we can expect that the transition will happen at $U = 0^+$ for the Baeriswyl wave function. Unfortunately, not much is known about the Baeriswyl wave function because even the calculation of the variational ground state energy is too difficult for general Hamiltonians. Below, we show how this can be accomplished for the $1/r$-Hubbard model. Our analysis will confirm our general considerations on the metal-to-insulator transition in this wave function.

Obviously, it is necessary to go beyond Gutzwiller and Baeriswyl wave functions because neither of them is able to describe the metal-to-insulator transition of the $1/r$-Hubbard model at $U = W$. Their natural generalization is the “Gutzwiller-Baeriswyl” wave function defined as

$$|\psi_{GB}(b, g)\rangle = b^{\hat{T}/W} g^{\hat{D}}|\text{Fermi-sea}\rangle$$

(14)
For $b = 1$ this wave function reduces to the Gutzwiller wave function (12), and to the Baeriswyl wave function (13) for $g = 0$. We now have a two-parameter wave function which allows for the competition of the “kinetic” Baeriswyl correlator and the “potential” Gutzwiller correlator. We might hope that this competition will result in a variational prediction of a metal-to-insulator at some finite critical value $U_{c}^{GB}$. We will see below that this is not the case. Instead, we again find $U_{c}^{GB} = \infty$ for the $1/r$-Hubbard model.

We denote $\langle \hat{O} \rangle = \langle \psi_{GB} | \hat{O} | \psi_{GB} \rangle / \langle \psi_{GB} | \psi_{GB} \rangle$. Details of the calculation are presented in appendix A. The final result for the expectation value of the kinetic energy is

$$\langle \hat{T}(b, g) \rangle / L = -\frac{W n(1 - n)}{4} + \frac{W}{8} \int_{-1}^{2n-1} dx \frac{\beta(x)^2 - \alpha(x)^2}{\beta(x)^2 + \alpha(x)^2}$$  \hspace{1cm} (15a)

and the mean double occupancy is given by

$$\langle \hat{D}(b, g) \rangle / L = \bar{d}(b, g) = \frac{1}{8} \int_{-1}^{2n-1} dx \frac{(\alpha(x)\sqrt{1 + x} + \beta(x)\sqrt{1 - x})^2}{\beta(x)^2 + \alpha(x)^2}$$  \hspace{1cm} (15b)

where

$$\alpha(x) \equiv \alpha(x; b, g) = \sqrt{\frac{1}{b}} \left[ 1 + \frac{g - 1}{2} (1 + x) \right]$$  \hspace{1cm} (16a)

$$\beta(x) \equiv \beta(x; b, g) = \frac{\sqrt{b}(g - 1)}{2} \sqrt{1 - x^2}$$  \hspace{1cm} (16b)

Before we proceed with the general case, we first discuss the special cases $b = 1$ (Gutzwiller wave function) and $g = 0$ (Baeriswyl wave function).

### A. Gutzwiller wave function

We set $b = 1$ in eqs. (15), (16), and obtain $\alpha(x; g) = [1 - x + g(1 + x)] / 2$, and $\beta(x; g) = (g - 1)\sqrt{1 - x^2}/2$. After some straightforward manipulations one arrives at

$$\bar{d}(g) = \frac{g^2}{2} \int_{0}^{\pi} dy \frac{y}{1 + (g^2 - 1)y}$$  \hspace{1cm} (17a)

$$\langle \hat{T}(g) \rangle / L = -\frac{W n(2 - n)}{4} + \frac{W}{2}(g - 1)^2 \int_{0}^{\pi} dy \frac{y(1 - y)}{1 + (g^2 - 1)y}$$  \hspace{1cm} (17b)
A simple integration gives

$$d(g) = \frac{g^2}{2(1-g^2)^2} \left[ -(1-g^2)n - \ln \left( 1 - (1-g^2)n \right) \right]$$

(18a)

$$\langle \hat{T}(g) \rangle / L = -\frac{Wn(2-n)}{4} - W \left( \frac{g-1}{g+1} \right) \left[ \left( \frac{n}{2} \right)^2 - d(g) \right]$$

(18b)

As shown in appendix B these results completely agree with those obtained from a direct application of the methods developed in Refs. [10,11], and provides an independent check for the conjectured solution of the 1/r-Hubbard model in Ref. [5].

To obtain the variational ground state energy density one has to minimize \( e_G^0(g) = \langle \hat{T}(g) \rangle / L + Ud(g) \) with respect to \( g \). This has to be done numerically for general \( U/W \).

The resulting curve at half-filling is shown in figure 2. It is seen that the Gutzwiller wave function is very good for values of \( U/W \leq 0.5 \). Indeed, as shown in appendix B, the Gutzwiller wave function gives the exact ground state energy to order \( U^2/W \) for all fillings. It is further exact to order \( n^3 \) for all values of \( U/W \), see appendix B. The logarithmic dependence of \( d(g) \) on \( g \) for small \( g \) (i.e., large \( U/W \)) causes the variational energy to behave like \( e_G^0 \sim W^2/|U \ln(U/W)| \), see Ref. [10], in contrast to the exact result, see eq. (11). As discussed in detail in Ref. [12], this wrong behavior of the variational ground state energy comes from the poor correlations between double occupancies and holes in the Gutzwiller wave function for large \( U/W \).

It is clearly seen that \( g > 0 \) for all \( U < \infty \) such that the variational prediction for the metal-to-insulator transition is \( U_c^G = \infty \). It should be clear, however, that at least the physics of this transition is correct: it is due to charge correlations, magnetic ordering neither occurs nor is it necessary. Furthermore, the transition only happens at \( n = 1 \) as it should, and not for arbitrary electron density as in the case of Hartree-Fock theory.

### B. Baeriswyl wave function

We know that the Gutzwiller-projected Fermi-sea is the exact ground state of the 1/r-tJ model with pair-hopping terms [38], i.e., of the Hamiltonian which one gets from eq. (1) by
first order perturbation theory in $W/U$. Consequently, the Baeriswyl wave function is the exact ground state of the $1/r$-Hubbard model (1) to order $W/U$ [17, 12].

For $g = 0$ the equations (16) can be simplified to
\[
\alpha(x; b) = \frac{1 - x}{2 \sqrt{b}} - \sqrt{b} \sqrt{1 - x^2}/2.
\]

After some straightforward manipulations eqs. (15) finally give
\[
\langle \hat{T}(b) \rangle / L = -\frac{W n (2 - n)}{4} + W \frac{b^2}{2 (1 - b^2)^2} \left[ - (1 - b^2) n - \ln \left( 1 - (1 - b^2) n \right) \right]
\]
\[
\overline{d}(b) = \frac{1 - b}{1 + b} \left[ - \frac{\langle \hat{T} \rangle / L}{W} - \frac{n (1 - n)}{2} \right] .
\]

Comparing eqs. (18a) and (19a), and eqs. (18b) and (19b), we note that the mean kinetic energy and the mean double occupancy just change their roles when we go from the Gutzwiller wave function to the Baeriswyl wave function. However, this only happens in the highly symmetric $1/r$-Hubbard model.

Form this equivalence it immediately follows that there is a metal-to-insulator transition for $n = 1$ in the Baeriswyl wave function at $U^B_c = 0^+$, i.e., this wave function is insulating at half-filling for all $U > 0$. While for large $U/W$ we obtain the exact result $\epsilon_0^B = -W^2/(12U) + O(W^3/U^2)$, the wave function gives only a poor estimate for the ground state energy density at small $U/W$. One obtains the Hartree contribution to first order, but there is, at half-filling, no contribution to second order in $(U/W)^2$. Instead, the correction is proportional to $(U^2/W) \ln(U/W)$.

At least for the $1/r$-Hubbard model we can thus conclude that it is as insufficient as the Gutzwiller wave function in the opposite regime of its obvious applicability. This unsatisfactory behavior might in part be due to the special model. Unfortunately, this wave function cannot be evaluated for other Hamiltonians away from $b \lesssim 1$.

### C. Gutzwiller-Baeriswyl wave function

For finite $b$ and $g$, the Gutzwiller-Baeriswyl wave function represents a metallic state. We first analyze whether we can have a metal-insulator transition at a finite value of $U/W$. 
The integrals in eqs. (15) can be done analytically. To properly take care of possible
singularities we write
\[
\langle \hat{T}(b,g) \rangle / L = -\frac{W n(2-n)}{4} + \frac{W}{2} b^2 (g-1)^2 \left( I^{(1)} - I^{(2)} \right) 
\]
(20a)
\[
2\tilde{d}(b,g) = [1 + b(g-1)]^2 \left( I^{(1)} - I^{(2)} \right) + (g-1)^2 (1-b)^2 \left( I^{(3)} - I^{(2)} \right) + g^2 I^{(2)} 
\]
(20b)
where
\[
I^{(m)} = \int_0^n dy \frac{y^m}{A(b,g)y^2 + B(b,g)y + 1} 
\]
(21)
with \(A(b,g) = (g-1)^2(1-b^2) \geq 0\), \(B(b,g) = 2(g-1) + b^2(g-1)^2 \leq 0\). The denominator
of the integrals \(I^{(m)}\) has zeros at \(z_{1,2} = (|B| \pm \sqrt{B^2 - 4A})/(2A)\). One can easily show that
\(z_1 \geq z_2 \geq 1\). This implies that there will be a singularity (metal-insulator transition) only
at half-filling (the upper limit of integration is \(n \leq 1\)), if \(z_2 = 1\). This can only be fulfilled,
if \(A(b,g) + B(b,g) + 1 = 0\), or \(g = 0\), in agreement with our general considerations.

We have to find out whether the variational procedure gives \(g = 0\) at some finite \(U_{cGB}\).
To this end we have to carefully analyze the limit \(g \to 0\). We can assume that \(b\) will not be
unity because this would correspond to the case \(U_{cGB} = \infty\). In the limit \(g \to 0\) we first note
that \(z_2 \to 1 + \mathcal{O}(g^2)\), \(z_1 \to 1/(1-b^2)\). Then, the combinations \(I^{(1)} - I^{(2)}\) and \(I^{(3)} - I^{(2)}\)
stay finite, and actually are of the order \(g^2 \ln g\). Also, \(I^{(2)}(b,g) \sim \ln g\) for small \(g\). If we now
expand \(e_{0GB}(b,g)\) around \(g = 0\), one finds
\[
e_{0GB}(b,g) = e_{0B}(b) + e_1(b)g + e_2(b)g^2 \ln g + \ldots 
\]
(22)
The first term in this expansion, \(e_1(b) = \partial e_{0GB}(b,g)/\partial g \bigg|_{g=0}\) exists because all singularities at
least of the order \(g^2 \ln g\). After some lengthy calculations we find
\[
e_1(b) = -\frac{W}{(1-b^2)^2} \left[ 1 - b^2 + 2b^2 \ln b \right] + U \left[ \frac{1 - b^2 - 2b \ln b}{(1 + b)^3} \right] . 
\]
(23)
Close to the transition we can minimize eq. (22) with respect to \(g\) which gives
\[
g \ln g = -\frac{e_1(b)}{2e_2(b)} . 
\]
(24)
Thus we know \( g(b) \) as a function of \( b \). We insert this into our expansion (22) and obtain

\[
e_{0}^{\text{GB}}(b) = e_{0}^{B}(b) + \frac{g(b)}{2}e_{1}(b)
\]

(25)

For given \( U/W \) we have to compare the minima of \( e_{0}^{\text{GB}}(b) \) at \( b_{0}^{\text{GB}} \) and of \( e_{0}^{B}(b) \) at \( b_{0}^{B} \). If we denote the difference in the variational ground state energy densities by \( \Delta e_{0} = e_{0}^{\text{GB}}(b_{0}^{\text{GB}}) - e_{0}^{B}(b_{0}^{B}) \), and let \( b_{0}^{\text{GB}} = b_{0}^{B} + \delta b \) we may write for small \( g \)

\[
\Delta e_{0} \approx e_{0}^{B}(b_{0}^{GB}) + \frac{g(b_{0}^{GB})}{2}e_{1}(b_{0}^{GB}) - e_{0}^{B}(b_{0}^{B})
\]

\[
\approx \left. \frac{\partial e_{0}^{B}(b)}{\partial b} \right|_{b_{0}^{GB}} (\delta b) + \frac{1}{2} \left. \frac{\partial^{2} e_{0}^{B}(b)}{\partial b^{2}} \right|_{b_{0}^{GB}} (\delta b)^{2} + \frac{g(b_{0}^{GB})}{2}e_{1}(b_{0}^{GB})
\]

(26)

\[
= \frac{1}{2} \left. \frac{\partial^{2} e_{0}^{B}(b)}{\partial b^{2}} \right|_{b_{0}^{GB}} (\delta b)^{2} + \frac{g(b_{0}^{GB})}{2}e_{1}(b_{0}^{GB})
\]

The first term in the expansion in \( \delta b \) vanished by definition of the variational minimum. Accordingly, the second derivative is positive. The energy \( e_{1}(b_{0}^{\text{GB}}) \) must be negative to allow for \( g > 0 \) in eq. (24).

Now we are in the position to decide from the results of the numerical minimization procedure whether \( \Delta e_{0} \) is bigger or less than zero. We essentially find that \( g(b_{0}^{\text{GB}}) = \mathcal{O}(\delta b) \), typically \( g = 4 \cdot 10^{-5} \), \( e_{1}(b_{0}^{\text{GB}}) = -\mathcal{O}(10^{-2}W) \), \( \delta b = 5 \cdot 10^{-5} \), and \( (\partial^{2} e_{0}^{B})/(\partial b^{2})(b_{0}^{B}) = \mathcal{O}(W) \) for \( U/W = 10 \). Hence, the negative term \( g(b_{0}^{GB})e_{1}(b_{0}^{GB}) \) easily overcomes the positive contribution \( (\delta b)^{2}(\partial^{2} e_{0}^{B})/(\partial b^{2})(b_{0}^{B}) \) by several orders of magnitude. For all \( U/W \) we have \( \Delta e_{0} < 0 \), i.e., the Gutzwiller-Baeriswyl wave function for finite \( g \) always wins over the Baeriswyl wave function (\( g = 0 \)). The metal-to-insulator transition again happens at \( U_{c}^{\text{GB}} = \infty \). We had to do this detailed analysis because the energies of the Baeriswyl and the Gutzwiller-Baeriswyl energy become numerically indistinguishable for values of \( U/W > 5 \).

In general, the variational ground state energy density is obtained from a numerical minimization of \( e_{0}^{\text{GB}}(b,g) = \langle \hat{T}(b,g) \rangle/L + U\overline{T}(b,g) \) with respect to \( b \) and \( g \). Given the fact that the Gutzwiller-Baeriswyl wave function becomes exact both for small and large \( U/W \) we obtain an excellent estimate for the ground state energy for all \( U/W \). We thus plot the relative deviation \( |(e_{0}^{\text{GB}} - e_{0})/e_{0}| \) from the exact ground state energy in figure 3.
maximum error is very small, about 1.6% around $U/W = 1$, and strongly decreases for larger and smaller values of the interaction.

The Gutzwiller-Baeriswyl wave function becomes exact both for small and for large $U/W$, and it gives an excellent estimate for the exact ground state energy density. However, it still misses the metal-to-insulator transition in the $1/r$-Hubbard model at $U_c = W$.

**IV. CONCLUSIONS**

In this work we investigated variational approaches to the exactly solvable $1/r$-Hubbard Hamiltonian. We found a two-parameter trial state, the Gutzwiller-Baeriswyl wave function, which becomes exact in both the weak and strong-coupling limit, and gives an excellent upper bound for the exact ground state energy. Yet it fails to reproduce the metal-to-insulator transition in the half-filled $1/r$-Hubbard model at $U_c = W$. Instead it predicts $U_{c}^{\text{GB}} = \infty$, just like the Gutzwiller wave function, $U_{c}^{\text{G}} = \infty$. On the other hand, the Baeriswyl wave function predicts $U_{c}^{\text{B}} = 0^+$, also in contradiction to the exact result.

We thus see that even very elaborate correlated wave functions are unable to reproduce the correct ground state physics of a one-dimensional model. However, the Gutzwiller-Baeriswyl wave function has to be considered an “excellent” wave function according to the “energy criterion”. This implies that the “energy criterion” is not very valuable, if one wants to draw conclusions about the ground state physics of a given Hamiltonian. This finding is supported by the fact that the results of the Gutzwiller Approximation to the Gutzwiller wave function are in qualitative agreement with the ground state physics of the $1/r$-Hubbard model even though there are considerable quantitative differences. The energy estimate is rather poor, and not even variationally controlled, but the basic physical concept that charge-correlations drive the transition at a finite interaction strength is properly incorporated in the approximation.

Antiferromagnetic Hartree-Fock theory always overestimates the role of spin-correlations in the metal-to-insulator transition while charge-correlations are neglected. Thus, there is
no correlation energy for small interactions, the transition takes place for all particle fillings, and a finite sublattice magnetization occurs. All three features are not present in the exact solution, in part due to the low dimensionality of our system. The physics of the metal-to-insulator transition which is predicted to happen at a finite $U_c^{HF} = W/2$ is solely a consequence of spin-correlations, contrary to the physics of the transition in the model. We know that charge-correlations drive the Mott-Hubbard metal-to-insulator transition, and spin-correlations are only residual effects. Thus, the Hartree-Fock picture is always a qualitatively wrong description of correlated Fermi systems.

The situation in higher dimensions is more promising for variational approaches. A successful theory of normal fluid $^3$He is based on the Gutzwiller wave function [20], evaluated in the limit of high dimensions where the Gutzwiller Approximation to the Gutzwiller wave function becomes exact [10,13]. In low dimensions, however, systems are Luttinger Liquids [23] rather than Fermi liquids. Charge-spin separation in such systems makes it difficult to write down qualitatively correct wave functions in terms of the original Fermion operators. Since charge-spin separation is common to many one-dimensional systems, it is doubtful whether one can write down successful Jastrow-Feenberg wave functions for correlated itinerant Fermion systems in low dimensions.

APPENDIX A: CALCULATION OF THE GROUND STATE ENERGY FOR CORRELATED WAVE FUNCTIONS

In ref. [5] we introduced an effective Hamiltonian description of the energy spectrum of the $1/r$-Hubbard Hamiltonian. We choose a basis in which $\hat{T}$ is diagonal, and represent states by putting hard-core bosons for spin ($\hat{s}_{K,\sigma}$) and charge ($\hat{d}_{K}$, $\hat{e}_{K}$) degrees of freedom onto each site $K$, $K = \Delta(m + 1/2)$ ($m = -L/2, \ldots, L/2 - 1$). They obey a hard core constraint, $\sum_\sigma \hat{n}^\sigma_{K,\sigma} + \hat{n}^d_{K} + \hat{n}^e_{K} = 1$ for each $K$. Each site is then occupied by one and only one of these four objects, $\uparrow$, $\downarrow$, $\bullet$, $\circ$ [24].

In this representation the Fermi-sea reads
\[ |\text{Fermi-sea} \rangle \equiv |[\uparrow \downarrow] \ldots [\uparrow \downarrow] \rangle_{K=0} \bigg| [\bullet \circ] \ldots [\bullet \circ] \bigg|_{K_F} \circ \ldots \circ \bigg) \]

where we assumed an even particle number, and \( K_F = \pi (2n - 1) \). To calculate the energy expectation value of the Gutzwiller-Baeriswyl wave function we only need to know how \( \hat{T} \) and \( \hat{D} \) act on the Fermi sea. From Ref. [5] we know that the kinetic energy operator can be split into two parts,

\[ \hat{T}_{\text{eff}}^0 = \sum'_{-\pi < K < \pi} \left\{ \frac{tK}{2} \left[ (\hat{s}_{K,\uparrow}^+ \hat{s}_{K,\uparrow} + \hat{s}_{K,\downarrow}^+ \hat{s}_{K,\downarrow}) - (\hat{d}_{K}^+ \hat{d}_{K} + \hat{e}_{K}^+ \hat{e}_{K}) \right] \right\} \quad (A1a) \]

\[ \hat{T}_{\text{eff}}^1 = \sum_{-\pi < K < \pi - \Delta} \lambda_K \pi t \left[ \hat{s}_{K,\uparrow}^+ \hat{s}_{K,\downarrow}^+ \hat{s}_{K+\Delta,\downarrow} \hat{s}_{K+\Delta,\uparrow} - \hat{d}_{K}^+ \hat{d}_{K} \hat{e}_{K+\Delta}^+ \hat{e}_{K+\Delta} \right] \quad (A1b) \]

where \( \lambda_K = \text{sgn}(K) \), and the prime on the sum in \( \hat{T}_{\text{eff}}^0 \) indicates that it must not be applied to the states represented by \( [\uparrow \downarrow] \) and \( [\bullet \circ] \) [5] which are treated separately by \( \hat{T}_{\text{eff}}^1 \). The total effective representation of the kinetic energy operator is \( \hat{T}_{\text{eff}} = \hat{T}_{\text{eff}}^0 + \hat{T}_{\text{eff}}^1 \).

The double occupancy operator is expressed by the two terms

\[ \hat{D}_{\text{eff}}^0 = \sum'_{-\pi < K < \pi} \hat{d}_{K}^+ \hat{d}_{K} \quad (A2a) \]

\[ \hat{D}_{\text{eff}}^1 = \sum_{-\pi < K < \pi - \Delta} \left\{ \frac{1}{2} + \lambda_K \frac{1}{4\pi} (2K + \Delta) \right\} \hat{d}_{K}^+ \hat{d}_{K} \hat{e}_{K+\Delta}^+ \hat{e}_{K+\Delta} \]

\[ + \left[ \frac{1}{2} - \lambda_K \frac{1}{4\pi} (2K + \Delta) \right] \hat{s}_{K,\uparrow}^+ \hat{s}_{K,\downarrow}^+ \hat{s}_{K+\Delta,\downarrow} \hat{s}_{K+\Delta,\uparrow} \]

\[ + \frac{1}{4\pi \sqrt{(2\pi)^2 - (2K + \Delta)^2}} \left[ \hat{d}_{K}^+ \hat{d}_{K+\Delta} \hat{s}_{K+\Delta,\uparrow} \hat{s}_{K+\Delta,\downarrow} + \text{H.c.} \right] \quad (A2b) \]

The total effective double occupancy operator is \( \hat{D}_{\text{eff}} = \hat{D}_{\text{eff}}^0 + \hat{D}_{\text{eff}}^1 \).

Fortunately, we only need to apply \( \hat{T}_{\text{eff}} \) and \( \hat{D}_{\text{eff}} \) to the Fermi-sea when we calculate the ground state energy of the Gutzwiller-Baeriswyl wave function. The states for \( K > K_F \) are already diagonal in \( \hat{T} \) and \( \hat{D} \), and just give an additive constant. We are left with the action of \( \hat{T}_{\text{eff}}^1 \) and \( \hat{D}_{\text{eff}}^1 \) which only act on neighboring pairs \([\uparrow \downarrow]\), and \([\bullet \circ]\) on \( K, K + \Delta \). We indicate this by a prime on the \( K \)-sums. For our purposes we may thus use the following matrix representation for \( \hat{T}_{\text{eff}} \)

\[ \hat{T}_{\text{eff}} = \sum'_{-\pi < K < K_F - \Delta} \hat{T}_{K,K+\Delta} + \sum_{K_F < K < \pi} \left( -\frac{tK}{2} \right) \quad (A3a) \]
\[ t_{K,K+\Delta} = t\pi \begin{pmatrix} \lambda_K & 0 \\ 0 & -\lambda_K \end{pmatrix} \]  

(A3b)

and for \( \hat{D} \):

\[ \hat{D}_{\text{eff}} = \sum'_{-\pi < K < K_F - \Delta} \hat{D}_{K,K+\Delta} \]  

(A4a)

\[ \hat{D}_{K,K+\Delta} = \frac{1}{2} \begin{pmatrix} 1 - \lambda_K a_K & \sqrt{1 - a_K^2} \\ \sqrt{1 - a_K^2} & 1 + \lambda_K a_K \end{pmatrix} \]  

(A4b)

where \( a_K = (2K + \Delta)/2\pi \). The matrix \( \hat{D}_{K,K+\Delta} \) has the eigenvalues zero and one.

We see that the problem of calculating expectation values \( \langle \hat{T} \rangle \) and \( \langle \hat{D} \rangle \) factorizes into independent \( 2 \times 2 \) matrix problems. We obtain

\[ \langle \hat{T} \rangle = \sum_{K_F < K < -\pi} \left( -\frac{tK}{2} \right) + \sum'_{-\pi < K < K_F - \Delta} \frac{\hat{\Lambda}_{K,K+\Delta} \hat{T}_{K,K+\Delta} \hat{\Lambda}_{K,K+\Delta}}{\hat{\Lambda}_{K,K+\Delta} \hat{\Lambda}_{K,K+\Delta}} \]  

(A5a)

\[ \langle \hat{D} \rangle = \sum'_{-\pi < K < K_F - \Delta} \frac{\hat{\Lambda}_{K,K+\Delta} \hat{D}_{K,K+\Delta} \hat{\Lambda}_{K,K+\Delta}}{\hat{\Lambda}_{K,K+\Delta} \hat{\Lambda}_{K,K+\Delta}} \]  

(A5b)

\( \hat{\Lambda}_{K,K+\Delta} \) is the transpose of the vector

\[ \hat{\Lambda}_{K,K+\Delta} = M_{K,K+\Delta} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \begin{cases} \text{for } -\pi < K < 0 \\ \text{for } 0 < K < K_F \end{cases} \]  

(A6)

with the “correlation matrix” \( (\hat{1} \text{ is the } 2 \times 2 \text{ unit matrix}) \)

\[ \hat{M}_{K,K+\Delta} = b^{t_{K,K+\Delta}/W} g^{\hat{D}_{K,K+\Delta}} \]

\[ = \begin{pmatrix} b^{\lambda_K/2} & 0 \\ 0 & b^{-\lambda_K/2} \end{pmatrix} \left( \hat{1} + (g - 1) \hat{D}_{K,K+\Delta} \right) \]  

(A7)

We thus get \( \hat{\Lambda}_{K,K+\Delta} = (\alpha(a_K; b, g) \beta(a_K; b, g)) \) for \(-\pi < K < 0\), and \( \hat{\Lambda}_{K,K+\Delta} = (\beta(a_K; b, g) \alpha(a_K; b, g)) \) for \(0 < K < K_F\) where \( \alpha(x; b, g) \) and \( \beta(x; b, g) \) were defined in eqs. (16).
Going from $K < 0$ to $K > 0$ we see that the two entries in $\Lambda_{K,K+\Delta}$ are exchanged. The same happens to row and columns in the Hamilton matrix $\hat{H}_{K,K+\Delta} = \hat{T} + U\hat{D}$ such that we may drop the distinction between the two cases. It now is a straightforward task to evaluate eqs. (A3) in terms of $\alpha(x;b,g)$ and $\beta(x;b,g)$. In the thermodynamical limit one easily arrives at eq. (15), if one takes into account that the primed sums give an extra factor of a half in front of the integral because only every second $K$-value has to be included.

APPENDIX B: ALTERNATIVE CALCULATION OF THE GROUND STATE ENERGY FOR THE GUTZWILLER WAVE FUNCTION

We want to directly calculate the ground state energy of the Gutzwiller wave function by using the methods of Vollhardt et al. [10,11]. To this end we first shift the Fermi-sea of filled states between $k = -\pi$ and $k_F = \pi(n-1)$ by $(\pi - k_F)/2$ to generate a symmetric Fermi body $\langle \tilde{n}_{k,\sigma}\rangle$. This transformation does not change the double occupancy operator. We may then directly apply all formulae of Refs. [10,11]. For example, the formula for the average double occupancy $\bar{d}(g)$ agrees with eq. (18a). To obtain the average kinetic energy we have to calculate $\sum_{k,\sigma} \epsilon[k-(\pi-k_F^c)/2] \langle \tilde{n}_{k,\sigma}\rangle$ where $\langle \tilde{n}_{k,\sigma}\rangle$ can recursively be obtained [10]. In our case we do not need such detailed information to calculate the average kinetic energy. We take the lattice periodicity of our dispersion relation into account, and write

$$\langle \hat{T}(g) \rangle = -\frac{t}{2}(\pi-k_F^c) \sum_{-\pi<k<\pi,\sigma} \langle \tilde{n}_{k,\sigma}\rangle + 2\pi t \sum_{-\pi<k<-\pi+(\pi-k_F^c)/2} \langle \tilde{n}_{k,\sigma}\rangle$$

(B1)

where we dropped the term $\sum_{-\pi<k<\pi,\sigma} tk \langle \tilde{n}_{k,\sigma}\rangle = 0$ which vanishes because the dispersion is antisymmetric but the shifted momentum distribution $\langle \tilde{n}_{k,\sigma}\rangle$ is symmetric around $k = 0$. The first $k$-sum in (B1) gives the total number of electrons while the second gives half the number of electrons outside the Fermi body, $n_{\text{out}}/2$, for which a closed expression can be given [10]

$$n_{\text{out}} = 2\frac{1-g}{1+g} \left[ \frac{n}{2} \right]^2 - \bar{d}(g)$$

(B2)
The average kinetic energy then indeed reduces to eq. (18b).

We will now show that the Gutzwiller wave function gives the exact ground state energy to order \((U/W)^2\). To this end we recall [5,8] that the energy spectrum of the kinetic energy operator for fixed total momentum consists of equidistant levels, separated by \(W\). The potential energy operator can be split into three parts: \(\hat{D}_0\) which commutes with \(\hat{T}\), and \(\hat{D}_\pm\) which scatter eigenstates of \(\hat{T}\) such that the final state has a by \(W\) higher (lower) kinetic energy. To first order in \(U/W\) we can write the (non yet normalized) exact ground state as

\[
|\psi_0\rangle = \left[1 + \alpha \hat{D}\right] |\text{Fermi-sea}\rangle
\]

with \(\alpha = \mathcal{O}(U/W)\) because the Fermi-sea is the unique ground state (the application of \(\hat{D}_0\) only gives the Fermi-sea again). This expression is nothing but the Gutzwiller wave function to order \((g−1)\) such that the two wave functions agree to first order in perturbation theory (the minimization procedure gives \(1−g = U/W\)). Consequently, the Gutzwiller wave function gives the exact ground state energy to order \((U/W)^2\) for the \(1/r\)-Hubbard model.

A similar line of arguments can be used to show that the Gutzwiller wave function also gives the exact ground state energy to order \(n^3\) for all \(U/W\). To this end, we recall that the exact ground state wave function for small densities is given by the Fermi sea and one particle-hole pair which is created by the action of \(\hat{D}_\pm\). For low densities only ladder-diagrams contribute which means that no further particle-hole pairs are created but only the existing one is scattered. This corresponds to the repeated action of \(\hat{D}_0\) in the subspace of the same kinetic energy. This means that all eigenstates of the kinetic energy operator which correspond to one particle-hole pair retain the same phase factor. To first order in \(n\) we may replace all operators \(\hat{D}_0, \hat{D}_\pm\) by \(\hat{D}\). It is thus seen that the exact wave function to first order in \(n\) has the same states with one particle-hole pair as the Gutzwiller wave function. In particular, these states have the same relative phases. Consequently, the Gutzwiller wave function is exact to the first non-trivial order in the density, and thus gives the exact ground state energy to order \(n^3\) for all interaction strength \(U/W\). The corresponding optimal value of \(g\) is \(g = 1/(1 + U/W)\).

We see that lowest-order perturbation theory for the \(1/r\)-Hubbard model is easily done
because the Gutzwiller wave function becomes exact in this limit.
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FIGURES

FIG. 1. Hartree-Fock ($e_0^{\text{HF}}$) and exact ($e_0$) ground state energy density at half-filling as function of $U/W$. For comparison we also include the result of the Gutzwiller Approximation to the Gutzwiller wave function, $e_0^{\text{GA}}$.

FIG. 2. Exact ($e_0$) and Gutzwiller/Baeriswyl ($e_0^G, e_0^B$) variational ground state energies as function of $U/W$ for the half-filled case; on this scale there is no distinction possible between the exact ground state energy density and the variational result from the two-parameter Gutzwiller-Baeriswyl wave function, $e_0^{\text{GB}}$.

FIG. 3. Relative error $| (e_0^{\text{GB}} - e_0) / e_0 |$ of the Gutzwiller-Baeriswyl variational energy, $e_0^{\text{GB}}$, compared to the exact ground state energy density, $e_0$, at half-filling.