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The Gutzwiller wave function as a disentanglement prescription

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Abstract. The Gutzwiller variational wave function is shown to correspond to a particular disentanglement of the thermal evolution operator, and to be physically consistent only in the temperature range $U \ll kT \ll E_F$, the Fermi energy of the non-interacting system. The correspondence is established without using the Gutzwiller approximation. It provides a systematic procedure for extending the ansatz to the strong-coupling regime. This is carried out to infinite order in a dominant class of commutators. The calculation shows that the classical idea of suppressing double occupation is replaced at low temperatures by a quantum RVB-like condition, which involves phases at neighboring sites. Low-energy phenomenologies are discussed in the light of this result.

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1 Introduction

Variational wave functions are a highly select class of results in the physics literature. There are only five which are widely used: Hartree-Fock and BCS for weak perturbations of the Fermi sea [1], Feynman's ansatz for the ground state of liquid ^{4}He [2], Laughlin's wave function for the fractional quantum Hall effect [3], and Gutzwiller's ansatz for the ground state of the Hubbard model [4]. The last two fall into the class of Jastrow wave functions [5], one of which was also used to describe ^{4}He and ^{4}He–^{3}He mixtures [6], and which are currently considered generic for strongly correlated problems.

Of these, Gutzwiller's is by far the least understood. Its underlying physical idea is that electrons of one spin see those of the other as a 'smeared background' [4]. This very drastic assumption is still not sufficient to provide an operational prescription, but is supplemented by another, the 'Gutzwiller approximation:' electrons of one spin see the others 'as if occupying a band of width zero' [4], i.e. their mass is taken to be infinite. This prescription was never given a justification from first principles in any finite dimension. It is true by construction when the number of dimensions approaches infinity [7], because the scaling of hopping overlaps, required to obtain finite results in that limit, makes all motion effectively diffusive.

The present work approaches Gutzwiller's wave function from a perspective not suggested by its variational origin. It turns out that it is based on a one-step Trotter decomposition of the thermal evolution operator, strictly valid only if the on-site repulsion U is much lower than the temperature. This insight provides a natural scheme for improvement. A direct implementation of it shows that Gutzwiller's prescription to remove double occupation is the first step in a transcedent series. When summed, it yields a new projector, which imposes a quantum condition with much stronger selectivity than the one removing double occupation. In the physical subspace satisfying this condition, Gutzwiller's program may be carried over to the strong-coupling regime $kT \ll t \ll U$ as well, where t is the hopping overlap. It can also be shown that at least at the level of expectation values, the on-site interaction does not scatter out of the new physical subspace. Unlike the requirement of no double occupancy, the quantum condition cannot be factorized into commuting local terms, indicating that relative phases on neighboring sites play an important role in the realization of the insulating ground state. The arguments are limited to the immediate vicinity of half-filling, where the configuration space for processes not considered here is small.

2 The Gutzwiller ansatz

Take the Hubbard Hamiltonian on a square lattice, $H = K + V$, where K is the kinetic term and $V = U \sum_i n_{i\uparrow} n_{i\downarrow}$. Define the operator $\mathcal{K}$ by a factorization of the imaginary-time evolution operator,

$$e^{-\beta(K+V)} \equiv e^{-\beta V/2} e^{-\beta \mathcal{K}} e^{-\beta V/2}. \tag{1}$$

The main result of this section is that the Gutzwiller ansatz neglects the entanglement of K and V. To prove

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this, take $\mathcal{K} = K$ and calculate the expectation with respect to any operator $\mathcal{O}$:

$$\frac{\text{tr } \mathcal{O}e^{-\beta V/2}e^{-\beta K}e^{-\beta V/2}}{\text{tr } e^{-\beta K}} = \frac{\sum_P \langle P| e^{-\beta V/2}\mathcal{O}e^{-\beta V/2}e^{-\beta K} |P\rangle}{\text{tr } e^{-\beta K}}$$
$$= \sum_{PRR'} \langle P|R\rangle \langle R| e^{-\beta V/2}\mathcal{O}e^{-\beta V/2} |R'\rangle \langle R'|P\rangle \frac{\langle P| e^{-\beta K} |P\rangle}{\text{tr } e^{-\beta K}}$$
$$= \sum_{RR'} \left[e^{-\beta U(D_R+D_{R'})/2} \langle R| \mathcal{O} |R'\rangle\right] \sum_P \frac{\langle P| e^{-\beta K} |P\rangle}{\text{tr } e^{-\beta K}} \times \langle R'|P\rangle \langle P|R\rangle . \quad (2)$$

Here $|P\rangle$ are momentum eigenstates, and $|R\rangle, |R'\rangle$ position eigenstates. Use has been made of the fact that K is diagonal in momentum, and V in position: $V|R\rangle = UD_R|R\rangle$, where D_R is the number of doubly occupied sites in configuration $|R\rangle$. Now perform the same calculation for the expectation value $\langle g| \mathcal{O} |g\rangle$ in Gutzwiller's wave function $|g\rangle = P(g)|\Psi\rangle$, with $|\Psi\rangle$ a non-interacting ground state and $P(g)$ the Gutzwiller projector:

$$P(g) = \prod_i [1 - (1-g)n_{i\uparrow}n_{i\downarrow}] \equiv \prod_i \left[\widehat{E}_i + \widehat{A}_{i\uparrow} + \widehat{A}_{i\downarrow} + g\widehat{D}_i\right], \quad (3)$$

where the hatted operators are projectors onto empty sites, sites occupied by a single spin (up or down), and doubly occupied sites, respectively [8]. Then

$$\langle g| \mathcal{O} |g\rangle = \sum_{RR'} \langle \Psi|R\rangle \langle R| P(g)\mathcal{O}P(g) |R'\rangle \langle R' |\Psi\rangle = \sum_{RR'} \left[g^{D_R+D_{R'}} \langle R| \mathcal{O} |R'\rangle\right] \langle R'|\Psi\rangle \langle \Psi|R\rangle , \quad (4)$$

remembering that $P(g)|R\rangle = g^{D_R}|R\rangle$. Now observe that the non-interacting ground state $|\Psi\rangle$ is itself a momentum eigenstate. The same term $P = \Psi$ will dominate the sum over P in equation (2), if one takes the temperature low enough. The expectation value (2) then reads

$$\text{tr } \mathcal{O}e^{-\beta^* V/2}e^{-\beta^* K}e^{-\beta^* V/2} \approx \sum_{RR'} \left[e^{-\beta^* U(D_R+D_{R'})/2} \langle R| \mathcal{O} |R'\rangle\right] \langle R'|\Psi\rangle \langle \Psi|R\rangle , \quad (5)$$

where β^* is a particular value of the temperature, for which the non-interacting system is in its ground state, to any desired accuracy.

We are led to the astonishing conclusion, that the result (5) of this procedure is the same as taking expectation values with respect to Gutzwiller's variational wave function, equation (4). The correspondence

$$\langle g| \mathcal{O} |g\rangle \leftrightarrow \text{tr } \mathcal{O}e^{-\beta^* V/2}e^{-\beta^* K}e^{-\beta^* V/2} \quad (6)$$

between the two expressions (4) and (5) is established simply by replacing

$$g \leftrightarrow e^{-\beta^* U/2}. \quad (7)$$

The fact that the denominator in equation (2) was tr $e^{-\beta K}$ and not (more logically) tr $e^{-\beta K}e^{-\beta V}$ is counterpart to the fact that $\langle g|g\rangle$ is not normalized. Taking $\mathcal{O} = 1$, it immediately follows that $\langle g|g\rangle \leftrightarrow$ tr $e^{-\beta K}e^{-\beta V}/$tr $e^{-\beta K}$ under the above correspondence.

The original calculation of Gutzwiller also contains a prescription to fix β^*, or g. This is to take $\mathcal{O} = H$, the Hamiltonian, and obtain g variationally. However, it is difficult to imagine such a procedure to compensate for the steps which were taken to arrive at Gutzwiller's form, equation (5). Neglecting entanglement to get from equation (1) to equation (2) requires $U \ll kT$, or more precisely, $Ut \ll (kT)^2$. This is the step usually made in the Trotter formula, for a single short 'slice' of the evolution integral, which is eventually taken to zero (i.e. the temperature to infinity). To single out the ground-state term in equation (2) and so obtain equation (5), requires, on the other hand, the temperature to be low, $kT \ll E_F$, the Fermi energy of the non-interacting ground state. The two are possibly consistent only in the range

$$U \ll kT \ll E_F, \quad (8)$$

which is not the strong-coupling regime $kT \ll t \ll U$, for which the Gutzwiller approach was intended.

On the other hand, in practice the expectation value (4) is usually calculated in the so-called Gutzwiller approximation, so it is desirable to understand its effect on the above derivation. It was shown in reference [8] that the approximation amounted to replacing the configurational overlaps by a constant,

$$\langle R'|P\rangle \langle P|R\rangle \to \frac{1}{\mathcal{N}}, \quad (9)$$

where $\mathcal{N}$ is the number of terms in the sum over configurations R, R'. Inserting this in equation (2) yields

$$\frac{1}{\mathcal{N}} \sum_{RR'} \left[e^{-\beta^* U(D_R+D_{R'})/2} \langle R| \mathcal{O} |R'\rangle\right], \quad (10)$$

which is the same as obtained from equation (4) with Gutzwiller's approximation, without invoking the limit $kT \ll E_F$. The physical role of the Gutzwiller approximation is clear now. Instead of neglecting the *excited* states in equation (2), as done above by going to low temperature, it neglects the *difference* between the ground and excited states. When all the terms $\langle R'|P\rangle \langle P|R\rangle$ are replaced by the constant $1/\mathcal{N}$, of course their thermal average in equation (2) reduces to this single constant term. One gets again the same result as if the ground-state term alone had been taken into account.

To summarize, calculating the expectation value of any operator with respect to Gutzwiller's wave function is exactly equivalent to the following three steps, when calculating its thermal expectation with respect to

$e^{-\beta(K+V)}$: first (a) neglect the entanglement of the potential and kinetic terms, so that one can replace

$$e^{-\beta(K+V)} \to e^{-\beta V/2} e^{-\beta K} e^{-\beta V/2}, \tag{11}$$

forgetting all commutators of V and K; then (b) take only the ground-state term from equation (2); finally (c) use a variational procedure to fix the left-over temperature-dependent parameter $e^{-\beta^* U/2} = g$, irrespective of consistency with the previous two steps. Needless to say, the first two steps are themselves hardly justifiable in the strong-coupling limit $U \gg t$.

3 Lowest-order improvement

In the previous section, it was shown that the expectation values calculated with the Gutzwiller ansatz can be obtained in a thermal formalism which neglects the entanglement of kinetic and potential energy terms. This is true irrespective of the use of the Gutzwiller approximation, which itself amounts to replacing the thermal average in equation (2) with a normalization constant. The whole procedure retains only a classical attenuation of double occupation, such that equation (1) is approximately valid with $\mathcal{K} = K$, i.e. all quantum dynamical correlations, coming from the commutators, are neglected. The main subject of the present work is to investigate the effect of the neglected commutators systematically.

Including the commutators amounts to adding quantum correlations to Gutzwiller's wave function, which should be present in the strong-coupling low-temperature state, $kT \ll t < U$. Technically, this boils down to finding a better expression for the operator $\mathcal{K}$ in equation (1). The reason $\mathcal{K} \neq K$ is that the commutator $[V, K]$ is not zero. Explicitly,

$$V^k \circ K = tU^k \sum_{\substack{\langle i,j\rangle \\ \sigma}} (n_{i,-\sigma} - n_{j,-\sigma})^k \times \left(a^\dagger_{i\sigma} a_{j\sigma} + (-1)^k a^\dagger_{j\sigma} a_{i\sigma} \right), \tag{12}$$

where t is the hopping overlap, and the operation $\circ$ is a commutator,

$$V^n \circ K \equiv \left[V, V^{n-1} \circ K \right] \tag{13}$$

with $V^0 \circ K \equiv K$. The vanishing of the commutator is obviously consistent with the original 'smeared background' interpretation, $n_{i,-\sigma} \to \langle n_{-\sigma} \rangle$. This points the way to an a posteriori justification of the Gutzwiller ansatz (though not of the Gutzwiller approximation). One can claim to work in a physical regime where it is sensible to replace the number operators by the average occupation of a site, as it should be in a doped metallic state, away from the metal-insulator transition. There one can hope that the high-temperature decomposition, equation (11), may in fact extend to low temperature.

In the remainder of this section, the effect of including a single additional commutator will be studied. It will be shown below that the commutator $[V, K]$ itself does not contribute to $\mathcal{K}$, because of the symmetry of the decomposition (1), so the lowest non-zero contributions to same order in β are $[V, [V, K]]$ and $[K, [V, K]]$. When $U \gg t$, the limit of interest here, the first is more important. Retaining only this one term,

$$\begin{aligned} \mathcal{K} &\to K + \frac{1}{6} \left(\frac{\beta}{2} \right)^2 [V, [V, K]] \\ &= t \sum_{\substack{\langle i,j\rangle \\ \sigma}} \left[1 + \frac{(\beta U)^2}{24} n_{ij,-\sigma} \right] \left(a^\dagger_{i\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{i\sigma} \right) \\ &\equiv K + K_1, \end{aligned} \tag{14}$$

where the numerical factors will also be justified later, and

$$n_{ij,-\sigma} = (n_{i,-\sigma} - n_{j,-\sigma})^2 = n_{i,-\sigma} + n_{j,-\sigma} - 2 n_{i,-\sigma} n_{j,-\sigma} \tag{15}$$

is equal to one if the hop changes the number of doubly occupied sites, and zero otherwise.

How can one use this result to improve Gutzwiller's ansatz? Note that the norm of Gutzwiller's wave function can be written

$$\langle \Psi | \, P(g) P(g) \, | \Psi \rangle \leftrightarrow \frac{\operatorname{tr} e^{-\beta V/2} e^{-\beta K} e^{-\beta V/2}}{\operatorname{tr} e^{-\beta K}} \tag{16}$$

under the formal correspondence of the previous section. Obviously, one can interpret this as

$$P(g) \leftrightarrow e^{-\beta V/2}. \tag{17}$$

To confirm the interpretation, recall the well-known alternative form [9] of writing the Gutzwiller projector (3),

$$P(g) = \exp \left[-\eta \sum_i n_{i\uparrow} n_{i\downarrow} \right] = g^{\sum n_{i\uparrow} n_{i\downarrow}}, \tag{18}$$

where $\eta = -\ln g$. But this is just the right-hand side of (17), under the correspondence (7).

Now, the additional commutator in equation (14) amounts to replacing K by $K + K_1$ in the numerator of (16). Since we have decided not to include any additional commutators, we may rearrange terms at will, and write

$$\frac{\operatorname{tr} e^{-\beta V/2} e^{-\beta K_1/2} e^{-\beta K} e^{-\beta K_1/2} e^{-\beta V/2}}{\operatorname{tr} e^{-\beta K}} \tag{19}$$

for the 'improved' right-hand side of (16). It is obvious how to write an improved left-hand side now. There should be an additional projector, sensitive to configurations in which a hop would change the number of doubly occupied sites. Calling it $P_1(g_1)$, one may write

$$P_1(g_1) \leftrightarrow e^{-\beta K_1/2}. \tag{20}$$

Explicitly,

$$\begin{aligned} P_1(g_1) &= \exp \left[-\eta_1 \sum_{\substack{\langle i,j\rangle \\ \sigma}} n_{ij,-\sigma} \left(a^\dagger_{i\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{i\sigma} \right) \right] \\ &= g_1^{\sum n_{ij,-\sigma} \left(a^\dagger_{i\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{i\sigma} \right)}, \end{aligned} \tag{21}$$

where $\eta_1 = -\ln g_1$, and the new variational parameter corresponds to

$$g_1 \leftrightarrow e^{-\beta^3 t U^2/48}. \tag{22}$$

Hence the (systematically) improved variational wave function is

$$|g, g_1\rangle = P_1(g_1)P(g)\,|\Psi\rangle\,. \tag{23}$$

The practical aspects of evaluating the projector (21) are beyond this article. One immediately obvious technical complication is, however, theoretically significant: the projector (21) cannot be written in the product form (3). The reason is formally that the individual terms in the sum in equation (21) do not commute. Physically, this means that even the first quantum correction to Gutzwiller's program for the one-band Hubbard model already involves the relative phases of fermions on neighboring sites. The importance of phases was already noticed in reference [10], where it was shown that if a projector *can* be factorized into commuting local terms, then it *cannot* produce physical insulating behavior. In the following, it will be argued that while the use of projectors to remove unwanted parts of configuration space may be perfectly valid, such projectors cannot be used automatically to define effective Hamiltonians.

4 Extension to all orders

In the previous section, it was shown that the first quantum correction to Gutzwiller's projection involves bond phases. This is a setback for the local approach, so one is naturally led to ask, how important that correction is. What is the range of validity, in temperature, of the original ansatz? As luck would have it, this question admits of a sharp answer, because the correlation embodied in K_1 (or P_1) above can easily be studied to all orders in β. Unfortunately, the answer is rather disappointing: the low-temperature regime is approached exponentially fast. This statement should be moderated insofar as we really have in mind the state near half-filling. As already noted, any argument establishing a 'smeared background' automatically justifies Gutzwiller's ansatz at all temperatures. On the other hand, in the vicinity of the metal-insulator transition, one expects an electron to be scattered many times for each step it takes: there is not enough propagation in space to average out the local density. Then (12) contains the dominant processes affecting kinetic motion near half-filling, when $U > t \gg kT$.

The resummation of all commutators in (12) does not introduce new correlations, because

$$(n_{i,-\sigma} - n_{j,-\sigma})^{2k} = (n_{i,-\sigma} - n_{j,-\sigma})^2 = n_{ij,-\sigma} \tag{24}$$

is independent of k. However, it will show how fast (in temperature) they become important, if one can calculate how these commutators enter $\mathcal{K}$. The linear terms in a Baker-Campbell-Hausdorff (BCH) formula can be obtained by standard tricks [11], to give

$$\mathcal{K} = \frac{\sinh\left(\frac{\beta V}{2}\right)}{\frac{\beta V}{2}} \circ K + \left(1 - \frac{\beta K}{2}\coth\frac{\beta K}{2}\right) \circ V + \mathcal{O}(\beta^4 K^2 V^2) \tag{25}$$

for the case of equation (1). (Some details are given in Appendix A.) The first term is now evaluated with the help of equation (12), remembering that the projector (24) may be taken outside the Taylor series. One obtains

$$\mathcal{K} = t \sum_{\substack{\langle i,j\rangle \\ \sigma}} [1 + s(\beta U) n_{ij,-\sigma}] \left(a^\dagger_{i\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{i\sigma}\right) + \mathcal{O}(\beta^2 K^2)$$
$$\equiv K + K_1 + \mathcal{O}(\beta^2 K^2). \tag{26}$$

where we have redefined K_1. The point is now that the function

$$s(\beta U) = \frac{\sinh\left(\frac{\beta U}{2}\right)}{\frac{\beta U}{2}} - 1 \tag{27}$$

grows exponentially with βU. The interpretation (22) of the variational parameter g_1 should be replaced by

$$g_1 \leftrightarrow e^{-\beta t\, s(\beta U)/2}. \tag{28}$$

The projector P_1 in equation (23) becomes important at least as soon as

$$s(\beta U) > 1, \tag{29}$$

when K_1 and K become competitive. This is a much sharper condition than intuitively expected. On the other hand, it is also non-linear, so the correction in (26) is only 4% for $kT = U$, and the condition (29) is first satisfied for $kT \approx U/4.4$. One may thus replace the lower limit of validity of Gutzwiller's ansatz by $U/4 \ll kT$ (say), but that is obviously not essential.

Comparing the interpretations (7) of Gutzwiller's parameter, and (28) of g_1, more can be said. When $s(\beta U) > U/t$, the new projector P_1 becomes more important than Gutzwiller's P. Thus the very-low-temperature regime $kT \ll U$ is completely dominated by P_1, unless t/U is exponentially small, which is not normally the case. (The limit $U/t \to \infty$ is discussed later on.) For $kT \ll t < U$, the wave-function $P_1(g_1)\,|\Psi\rangle$ represents reality much better (exponentially better, to coin a phrase) than $P(g)\,|\Psi\rangle$. The strong-coupling limit is denoted $t < U$ rather than $t \ll U$ to avoid confusion with the limit $U/t \to \infty$, because we need $s(\beta U) \gg U/t$ when $kT \ll U$. However, U/t is always taken to be sufficiently large to relegate the neglected commutators to weak perturbations. Note that, since $s(\beta U)$ rises exponentially, such a regime is easily achieved. For example, for $kT = t/10 \ll t < U = 10t$, one gets

$$s(\beta U) = s(100) \sim 10^{19} \gg U/t = 10.$$

The formal reason for the overwhelming dominance of P_1 at low temperature is that the iterated commutator of Hubbard's contact interaction is non-zero to all orders. By comparison, for the harmonic oscillator already

the third iterated commutator vanishes: $[\hat{x}^2,[\hat{x}^2,\hat{p}^2]] \sim \hat{x}^2$, and similarly when $\hat{x}$ and $\hat{p}$ are interchanged. If all possible commutators are arranged in a table, such that the (n,m) cell collects those of order V^nK^m, this table is tridiagonal for the harmonic oscillator, while the expression (12) gives the first column for the contact interaction.

The final question in this section is about the relevance of the other commutators in the above-mentioned table, of which so far only the first column was treated. At kth order in β, commutators contribute which are of order $K^mV^{k-m} \sim t^mU^{k-m}$. The first column, summed completely by the hyperbolic sine in equation (25), contains all terms with $m=1$, i.e. like tU^{k-1}, while the other columns refer respectively to $1<m<k$. Thus at any given order in β, the term contained in the hyperbolic sine can be made to dominate those left out simply by increasing U/t. However, one should not hastily conclude that projectors generated by these terms are dominated by P_1 at low temperature in the same sense as Gutzwiller's $P(g)$. Like P_1, they are expected to have hyperbolic terms in βU in the exponent, where P is only linear in βU. Thus they should be relatively mildly suppressed with respect to P_1, by a power of the ratio t/U. However, since suppression by P_1 is the strongest, the configuration space determined by this projector alone is the largest one that needs to be taken into account, at least in the vicinity of half-filling.

5 The physical subspace

Looking back at the wave function (23), in the light of the underlying dependence (28) of g_1 with temperature, one may well wonder: what will survive such a projector at low temperature? Even if a wave function has a very small component to which K_1 in (26) is sensitive, the hyperexponential suppression by P_1 will annihilate it. The way out is obvious: the physically admissible space is the null-space of the operator K_1, $K_1|\Phi\rangle = 0$, or equivalently

$$[V,[V,K]]\,|\Phi\rangle = tU^2 \sum_{\substack{\langle i,j\rangle \\ \sigma}} n_{ij,-\sigma}\left(a^\dagger_{i\sigma}a_{j\sigma}+a^\dagger_{j\sigma}a_{i\sigma}\right)|\Phi\rangle = 0. \tag{30}$$

This gives a precise meaning to the 'smeared background' condition at low temperature and near half-filling, where it cannot be trivially satisfied by the replacement $n_{ij,-\sigma}\to 0$. A more careful formulation of the same idea is

$$\exp\left[-\beta(K+K_1)\right]|\Phi\rangle = \exp\left(-\beta K\right)|\Phi\rangle\,. \tag{31}$$

However, K_1 dominates K at low temperature because of the relative factor $s(\beta U)$, so one expects the physics to be contained in equation (30) by itself. One may be tempted to add the condition

$$V\,|\Phi\rangle = 0, \tag{32}$$

which is the no-double-occupancy constraint, but that is not warranted: for example, should the conditions (30) and (32) turn out to be incompatible, the discussion in the previous section shows that the system will choose (30) at low temperature. By the same token, the subdominant correlations, coming from the neglected commutators, may have a say in which combination of the states $|\Phi\rangle$ turns out to be the ground state, but they cannot enlarge the physical subspace any more than the no-double occupancy constraint: P_1 acts too stringently for that (if it does not, decrease the temperature, and/or increase the ratio U/t). If we decide to neglect all commutators containing at least two K's, such as $[K,[V,K]]$, because they are suppressed by at least t/U, the thermal expectation value in the physical subspace may be written at low temperature

$$\mathrm{tr}\,\mathcal{O}e^{-\beta V/2}e^{-\beta K+K_1}e^{-\beta V/2} = \sum_{\Phi}\langle\Phi|\,e^{-\beta V/2}\mathcal{O}e^{-\beta V/2}e^{-\beta K}\,|\Phi\rangle\,, \tag{33}$$

because the wave-functions which do not satisfy (30) have been eliminated by the projector P_1, while the admissible ones allow the simplification (31). This has formally the same structure as if we had made the high-temperature disentanglement (11), i.e. used Gutzwiller's scheme. However, the underlying physical regime is at low temperature and strong coupling, ensured by the requirement (30) on the states $|\Phi\rangle$.

If $U/t\to\infty$, the dominance of P_1 over Gutzwiller's P cannot be established quantitatively. This does not invalidate the former reasoning, but merely opens the possibility that the physical subspace is further reduced in the calculation (33). However, there is a qualitative argument that Hubbard's interaction leaves the physical subspace invariant. Namely, the identity

$$VAV = \frac{1}{2}\left(V^2A + AV^2 - [V,[V,A]]\right) \tag{34}$$

holds for any operators V and A. Now take V to be Hubbard's repulsion, and $A=[V,[V,K]]$, cf. equation (30). Let $|\Phi\rangle$ be a state satisfying equation (30), i.e. $A|\Phi\rangle = 0$. Then the state $V|\Phi\rangle$ also satisfies equation (30), at the level of expectation values:

$$\langle\Phi|\,VAV\,|\Phi\rangle = -\frac{1}{2}\langle\Phi|\,[V,[V,A]]\,|\Phi\rangle \propto \langle\Phi|\,A\,|\Phi\rangle = 0, \tag{35}$$

because $[V,[V,A]]\propto A$, by virtue of (12) and (24). In other words, Hubbard's repulsion does not on the average scatter out of the null-space defined by equation (30). This is strong indication that the latter has been correctly identified as the physical subspace.

6 Effective Hamiltonians

In the previous section, the physical subspace (30) was found to have two important properties. One, it is on the average invariant to V. Two, within it Gutzwiller's disentanglement ('smeared background') holds, so that hopping proceeds by the bare operator K, cf. equation (31). This

should be contrasted with the no-double-occupancy subspace, which is strongly perturbed by K, requiring the introduction of projected hopping

$$\widetilde{K} = t \sum_{\substack{\langle i,j \rangle \\ \sigma}} (1 - n_{i,-\sigma})\, a^{\dagger}_{i\sigma} a_{j\sigma}\, (1 - n_{j,-\sigma}) + \text{h.c.}, \qquad (36)$$

to keep within it. Both schemes take into account that an electron cannot hop locally onto anything but an empty site, in which case it tunnels by the full overlap t. In the first one, the burden of accounting for these dynamical correlations is taken by the construction (30) of the physical subspace, while in the no-double-occupancy scheme it is carried by the projected-hopping operator $\widetilde{K}$.

To compare the two clearly, note that using the projected-hopping operator in the no-double-occupancy subspace amounts to the calculation of thermal traces of the type

$$\text{tr}\ \mathcal{O} e^{-\beta V/2} e^{-\beta \widetilde{K}} e^{-\beta V/2} \qquad (37)$$

at arbitrarily low temperature. Now, the *exact* expression for the trace is

$$\text{tr}\ \mathcal{O} e^{-\beta(K+V)} = \text{tr}\ \mathcal{O} e^{-\beta V/2} e^{-\beta \mathcal{K}} e^{-\beta V/2}, \qquad (38)$$

by the definition (1) of the operator $\mathcal{K}$. As shown in the previous sections, the relevant part of $\mathcal{K}$ at low temperature is $K + K_1$, which in turn reduces either to K_1 in the unphysical subspace (since $K_1 \gg K$ there), or to K in the physical subspace, defined to be the null-space of K_1. Even if this separation into physical and unphysical subspaces turned out to be wholly misguided, still the fact would remain, that $\mathcal{K}$ has no component of the type $\widetilde{K}$. The neglected commutators cannot change this, because (a) they can be independently suppressed, simply by increasing the ratio U/t, and (b) they contain K at least twice, as in $[K,[V,K]]$, so they generate three-site and spin-exchange correlations, which are absent in $\widetilde{K}$.

In fact even more can be said: neither the classical constraint (32), nor the quantum constraint (30) can be used to define an effective Hamiltonian. The reason is that they are both *negative* statements, excluding some unwanted correlations. An effective Hamiltonian, on the other hand, acts to build up desirable correlations, not to reject undesirable ones. For example, the Hartree-Fock Hamiltonian has the respective Slater determinant as its ground state. By contrast, the null-space conditions (30) or (32) give no indication, which combination of states satisfying them is quasi-stationary with respect to the Hubbard Hamiltonian. Having an effective Hamiltonian is equivalent to knowing the approximate (saddle-point) equation of motion within the physical subspace, which is much more than knowing which states are not in that subspace.

There is a simple and rather dramatic way to emphasize that null-space conditions are not equations of motion — or, equivalently, that projectors are not effective Hamiltonians. Within its regime of validity, one should be able to use an effective Hamiltonian H_{eff} just as if it were fundamental, i.e. forgetting that its elementary degrees of freedom have an internal structure. In particular, the same H_{eff} should be used in real and imaginary time. This reflects the requirement that the effective equations of motion admit the ensemble construction, i.e. are thermalized in the usual sense. Now, what is the real-time analogue of $K + K_1$, equation (26)? It is found by taking $\beta = i\tau$ in the function $s(\beta U)$,

$$s(i\tau U) = \frac{\sin\left(\frac{\tau U}{2}\right)}{\frac{\tau U}{2}} - 1. \qquad (39)$$

Note the different dependence on U. To drive the point home, consider the limit $\tau U \to \infty$. Then $s \to -1$, and

$$K + K_1 \to t \sum_{\substack{\langle i,j \rangle \\ \sigma}} \Big[(1 - n_{i,-\sigma}) a^{\dagger}_{i\sigma} a_{j\sigma} (1 - n_{j,-\sigma}) + (\text{h.c.}) \Big] + t \sum_{\substack{\langle i,j \rangle \\ \sigma}} \Big[n_{i,-\sigma} a^{\dagger}_{i\sigma} a_{j\sigma} n_{j,-\sigma} + (\text{h.c.}) \Big] \qquad (40)$$

because the projector which appears may be rewritten:

$$1 + s(i\tau U)\, n_{ij,-\sigma} \to 1 - n_{ij,-\sigma} = (1 - n_{i,-\sigma})(1 - n_{j,-\sigma}) + n_{i,-\sigma} n_{j,-\sigma}.$$

The first term in equation (40) is just the projected-hopping operator $\widetilde{K}$, while the second makes the whole expression particle-hole symmetric. The appearance of $\widetilde{K}$ under these conditions is direct evidence that it is not an effective Hamiltonian for the one-band Hubbard model. If it were, it could be used in imaginary time as well, while it was shown above that the correct imaginary-time expression is equation (26), not $\widetilde{K}$.

The formal way out of this real/imaginary time conundrum is again to work in the subspace (30), since the kinetic operator then reverts to the microscopic (bare) K on both axes. However, that is not the same as having an effective Hamiltonian. The prescription (33) correctly transcribes Gutzwiller's calculational framework to the regime $kT \ll t < U$, but this is at best the first step in finding the normal modes, still far from revealing them.

7 Discussion

The standard operator approach to an effective theory without double occupation is to find a similarity transformation [9,12]

$$SHS^{-1} = H_{\mathit{eff}} + \ldots, \qquad (41)$$

such that H_{eff} does not couple to the doubly occupied states to some given order, and truncate the remainder, represented above by dots. The present paper observes that such a procedure does not of itself guarantee a physical effective Hamiltonian. In particular, it is shown that avoiding double occupation is a semiclassical perception of the electron's behavior at strong coupling, which does not carry over to low temperature near half-filling. Imposing

null-space conditions does not imply there exist thermodynamically stable normal modes which satisfy them. If the approximate normal modes are known, it may indeed be possible to connect effective Hamiltonians with low-lying states written in projector form, as in the cases of Hartree-Fock and BCS. If they are not, using the connection by formal analogy runs into trouble, such as not having the same effective Hamiltonian on the real and imaginary time axes. In other words, while an equation of motion may be written as a null-space condition, $(H-E)\left|\Psi\right\rangle = 0$, not all null-space conditions are admissible constraints to some given equations of motion. Put more simply, fixing both the force and the effective constraint due to that force generally amounts to overspecifying the problem. To be certain the two are compatible is almost the same as knowing the solution.

The projected-hopping operator $\widetilde{K}$ is a case in point, since it appears in the literature in two different contexts. On the one hand, it may be derived by formal arguments based on (41), guided by the wish to avoid some parts of configuration space. On the other, the same $\widetilde{K}$ can be obtained by physical arguments from a more general three-band model, where it is claimed to describe the propagation of excitations against the background of a particular mode, the Zhang-Rice singlet [13]. In this case, the use of $\widetilde{K}$ as a true effective Hamiltonian depends only on whether the correct hierarchy of background, excitation, and thermalization time scales is established. The point is that one cannot derive an effective Hamiltonian without some image of a physical mode which becomes quasi-stationary under the action of the original one. The same is true in the variational context. For example, in his description of ^{3}He–^{4}He mixtures [6], McMillan checked that the Jastrow wave function for the ^{4}He background reduced in the long-wavelength limit to the density oscillations characterizing Feynman's formulation [2].

There is nothing wrong, in principle, with using projector language to guess properties of the solution, i.e. to try and delimit the physical subspace. This is the essence of Gutzwiller's program, which the present work expands systematically. It is shown here that the original program is (at best) consistent in the physical regime $U \ll kT \ll E_F$, and that it may be carried over to the regime $kT \ll t < U$ formally very simply, by working in the null-space of the 'most troublesome' commutator, equation (30). This was identified with the physical subspace in the low-temperature, strong coupling limit, by a projection argument: states which are not in this null-space were found to be hyperexponentially suppressed at low temperature, much more strongly than states containing double occupation. The question may of course be raised, whether keeping the simplification of Gutzwiller's disentanglement at low temperature is worth the price of working with the condition (30). In effect, the preservation of disentanglement has replaced avoiding double occupation as a guiding principle for the construction of the physical subspace. This requirement is at least consistent between real and imaginary time, but it remains to be seen whether it is compatible as a constraint with the microscopic on-site repulsion. Physically, it amounts to the conjecture that low-lying excitations in the Hubbard model near half-filling can be mapped onto an effective semiclassical gas. It is encouraging for this point of view that the on-site repulsion does not on the average scatter out of the new physical subspace.

The condition (30) is the first precise quantum formulation of Gutzwiller's 'smeared background' assumption. Its most interesting aspect is the role of phases. Indeed the expression indicates that the admissible physical states should be coherent, as suggested by the resonating-valence-bond (RVB) arguments of Anderson [14]. This should be contrasted with the viewpoint, based on the no-double-occupancy condition (32), that the system is insulating because the electron *locally* has difficulty overcoming the repulsion U. The latter leads to an essentially diffusive view of the Mott state, which was shown already in reference [10] not to give physical insulating behavior, precisely because it is incoherent, i.e. insensitive to relative phases on neighboring sites. The fact that the interaction loses coherence, $[K,V]=0$, as soon as $n_{ij,\sigma}=0$, then implies that the ground-state of the one-band Hubbard model is likely to be antiferromagnetic at half-filling, even at arbitrarily large U/t. This conjecture is specific to the one-band model, since $n_{ij,\sigma}$ appears in the commutator only because both sites, connected by the hopping, are subject to the local repulsion.

While this article was under review, new evidence appeared that the no-double-occupancy condition is not satisfied at low temperature in the one-band Hubbard model [15]. It turns out that the upper Hubbard band participates coherently in the low-energy density of states at half-filling, even for U/t as large as 12.

To conclude, it has been shown that the Gutzwiller variational ansatz is physically consistent only in the regime $U \ll kT \ll E_F$, inapplicable to the Mott transition. In the regime $U > t \gg kT$, the no-double-occupancy condition is replaced by a quantum condition (30), sensitive to local phases, which defines the physical subspace. Within this subspace, Gutzwiller's disentanglement scheme is recovered in the low-temperature, strong coupling limit as well. However, as always, one cannot find an effective Hamiltonian without knowing the dominant slow modes. The quantum projection (30) is hopefully a step forward in understanding their microscopic structure, but is not an equation of motion.

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Appendix A: Derivation of the first term in equation (25)

Let A and B be two algebraic indeterminates. Define

$$X = \ln\left(e^{A+B}e^{-A}\right),\ Y = \ln\left(e^{-A}e^{A+B}\right). \qquad \text{(A.1)}$$

It may be shown [11] that the parts linear in B of these expressions are

$$X \equiv_{\mathrm{B}} \frac{e^A - 1}{A} \circ B = X_B,\ Y \equiv_{\mathrm{B}} \frac{1 - e^{-A}}{A} \circ B = Y_B, \quad \text{(A.2)}$$

where the notation $\equiv_{\mathrm{B}}$ means 'equal up to terms linear in B', and the circle operation is a commutator, like in (13). The linear parts are called X_B and Y_B, as noted. Now

$$\begin{aligned} \ln\left(e^{-A}e^{2A+2B}e^{-A}\right) &= \ln\left(e^Y e^X\right) \\ &\equiv_{\mathrm{B}} \ln\left(e^{Y_B}e^{X_B}\right) \equiv_{\mathrm{B}} X_B + Y_B, \end{aligned} \quad \text{(A.3)}$$

where the second step is legal because neither X nor Y contain terms of order zero in B, and the third is trivial, since both X_B and Y_B are linear in B. Adding X_B and Y_B, one obtains

$$\ln\left(e^{-A}e^{2A+2B}e^{-A}\right) \equiv_{\mathrm{B}} \frac{e^A - e^{-A}}{A} \circ B. \quad \text{(A.4)}$$

This gives the first term in equation (25), putting $A = -\beta V/2$ and $B = -\beta K/2$.

For completeness, here is the derivation of (A.2) from reference [11]. First, introduce a convenient notation for left- and right-multiplication by A,

$$LB = AB,\ RB = BA, \quad \text{(A.5)}$$

so that, for instance, the commutator with A is written $(L - R)B$. Then one can write $A^pBA^q = L^pR^qB$, whence it is trivial to show

$$e^ABe^{-A} = e^Le^{-R}B = e^{L-R}B = e^A \circ B, \quad \text{(A.6)}$$

reverting to the circle notation. In the same vein,

$$\begin{aligned} (A+B)^n &\equiv_{\mathrm{B}} A^n + \sum_{k=0}^{n-1} A^kBA^{n-1-k} \\ &= A^n + \sum_{k=0}^{n-1} L^kR^{n-1-k}B, \end{aligned} \quad \text{(A.7)}$$

so that the factorization formula

$$(L - R)\sum_{k=0}^{n-1} L^kR^{n-1-k} = L^n - R^n \quad \text{(A.8)}$$

yields

$$A \circ (A+B)^n \equiv_{\mathrm{B}} (L^n - R^n)B = A^nB - BA^n, \quad \text{(A.9)}$$

from which follows the useful expression

$$A \circ e^{A+B} \equiv_{\mathrm{B}} e^AB - Be^A, \quad \text{(A.10)}$$

upon summation over n.

To get (A.2), first note that $X \equiv_{\mathrm{B}} X_B$ (no zeroth-order term), hence $e^X \equiv_{\mathrm{B}} 1 + X_B$. Then

$$\begin{aligned} A \circ X_B &\equiv_{\mathrm{B}} Ae^X - e^XA = Ae^{A+B}e^{-A} - e^{A+B}e^{-A}A \\ &= \left(Ae^{A+B} - e^{A+B}A\right)e^{-A} \equiv_{\mathrm{B}} \left(e^AB - Be^A\right)e^{-A} \\ &= e^ABe^{-A} - B = \left(e^A - 1\right) \circ B, \end{aligned} \quad \text{(A.11)}$$

where (A.10) and (A.6) were used in succession. This means that in order to get X_B itself, we need one less commutator in each term on the right-hand side. In the circle notation, this is just

$$X_B = \frac{e^A - 1}{A} \circ B, \quad \text{(A.12)}$$

which is the first expression in (A.2). The second is obtained in exactly parallel fashion.

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