Gossamer metals

Marcus Kollar
Institut für Theoretische Physik, Johann-Wolfgang-Goethe-Universität Frankfurt, Robert-Mayer-Straße 8, D-60054 Frankfurt am Main, Germany.
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Laughlin’s construction of exact gossamer ground states is applied to normal metals. We show that for each variational parameter $0 \leq g \leq 1$, the paramagnetic or ferromagnetic Gutzwiller wave function is the exact ground state of an extended Hubbard model with correlated hopping, with arbitrary particle density, non-interacting dispersion, and lattice dimensionality. The susceptibility and magnetization curves are obtained, showing that the Pauli susceptibility is enhanced by correlations. The elementary quasiparticle excitations are gapless, except for a half-filled band at $g = 0$, where a Mott transition from metal to insulator occurs.

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Progress in the understanding of many-body effects in strongly correlated electron systems, such as quantum magnets, narrow-band transition metal compounds, fractional quantum Hall systems, or high-temperature superconductors, has depended on a variety of theoretical tools. Important information about the electronic structure can often be obtained from ab initio calculations, which are however less reliable if interactions between electrons are dominant over their kinetic energy. On the other hand, the study of idealized model systems, containing only the presumably relevant degrees of freedom, can provide insight into microscopic physical mechanisms. However, since such models are rarely exactly solvable, analytical and numerical calculations usually involve approximations or extrapolations. In view of these limitations, support for proposed physical notions has occasionally come from an inverse strategy: starting from a correlated many-body wavefunction one constructs a hopefully “reasonable” model Hamiltonian for which it is the exact ground state. Correlated quantum phases may then be classified according to their elementary excitations or correlation functions. This approach has been useful in particular for the understanding of the fractional quantum Hall effect, spin-Peierls or Haldane-gap antiferromagnets, and quantum rotors.

Recently, Laughlin developed a new approach to high-temperature superconductivity, viewing the insulating state as a superconductor with very low superfluid density. Pursuing the above strategy, he proposed that the ground-state wavefunction of such a “gossamer superconductor” is obtained from the BCS mean-field product state by applying the Gutzwiller correlation operator $(0 \leq g \leq 1)$,

$$
\hat{K}(g) = g \sum_{\sigma} \hat{D}_{i\sigma} = \prod_{i} \left[ 1 - (1 - g) \hat{D}_{i} \right],
$$

where $\hat{D}_{i} = \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ is the operator for double occupation at lattice site $i$, and constructed a corresponding model Hamiltonian. Elementary excitations, the transition from superconductor to Mott insulator magnetic instabilities, and related mean-field Hamiltonians were also studied in this context.

The purpose of this letter is the application of Laughlin’s gossamer paradigm to normal metals, i.e., itinerant electrons on a lattice without broken (discrete) translational symmetries. (In particular, antiferromagnetic or superconducting phases are excluded.) It is well known that a metallic system can be driven into an insulating state by strong electronic correlations. This type of transition from metal to insulator, the Mott transition, occurs for example in transition metal oxides, and has been analyzed by a variety of theoretical methods. These include the variational Gutzwiller wavefunction (GWF) obtained by acting with on an uncorrelated Fermi sea. In general the GWF describes a correlated metal, except for the insulating state with one inmobile particle at each lattice site that results at $g = 0$ for a half-filled band. When used as a variational wavefunction for the Hubbard model and evaluated within the Gutzwiller approximation, this Brinkman-Rice (BR) transition occurs at finite critical Hubbard interaction $U_{c}^{BR}$. While the Gutzwiller approximation becomes exact in the limit of infinite dimensions, the BR transition is shifted to $U_{c}^{BR} = \infty$ in finite dimensions. However, the reliability of these variational results is limited, as the true ground state of the Hubbard model in infinite dimensions may behave rather differently; for example the number of doubly occupied sites in general does not vanish at the transition as in the BR scenario. Furthermore, the analysis of elementary excitations is hampered by the fact that the true ground state is lower in energy, and on these grounds the GWF has been criticized as inadequate for describing the Mott transition. Some of these difficulties are resolved for models with exact GWF ground states, which we now proceed to construct.

Metallic gossamer ground state. In general a gossamer ground state is built as follows. Starting from an uncorrelated product wave function $|\phi\rangle$ and operators $\hat{b}_{k\sigma}$ such that $\hat{b}_{k\sigma} |\phi\rangle = 0$ for all $k$ and $\sigma$, one applies an invertible many-body correlator $\hat{K}$ to obtain a correlated...
wavefunction $|\psi\rangle = \hat{K} |\phi\rangle$, and defines $\hat{b}_{k\sigma} = \hat{K} \hat{b}_{k\sigma} \hat{K}^{-1}$. Then $|\psi\rangle$ is an exact ground state of the hermitian Hamiltonian $\hat{H} = \sum_{k\sigma} \hat{E}_{k\sigma} \hat{b}_{k\sigma}^\dagger \hat{b}_{k\sigma}$ for arbitrary $\hat{E}_{k\sigma} \geq 0$, since $\hat{H} \geq 0$ and $\hat{H} |\psi\rangle = 0$.

In the present context we use the Gutzwiller correlator \[ as in Refs. 2, 3, 4, which is invertible for $g \neq 0$, $K(g)^{-1} = \hat{K}(g^{-1})$, but start from a product state containing spin-up and spin-down fermions, characterized by the occupation numbers $n_{0\sigma}^k$ (with $n_{0\sigma}^k = 0$ or 1),

$$\langle \phi \rangle = \prod_{k\sigma} (n_{0\sigma}^k + 1) \hat{c}_{k\sigma}^\dagger |0\rangle. \quad (2)$$

This state is annihilated by the operators $\hat{b}_{k\sigma} = (1 - n_{0\sigma}^k) \hat{c}_{k\sigma} + n_{0\sigma}^k \hat{c}_{k\sigma}^\dagger$. After some algebra, we can rewrite the Hamiltonian $\hat{H}$ as

$$\hat{H} = \hat{H}_t + \hat{H}_h + \hat{H}_U + \hat{H}_X + \hat{H}_Y + \text{const}, \quad (3)$$

$$\begin{align*}
\hat{H}_t & = \sum_{ij\sigma \tau} T_{ij\sigma \tau} \hat{c}_{ij\sigma}^\dagger \hat{c}_{ij\tau}, \\
\hat{H}_h & = \hbar \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}), \quad (4)
\end{align*}$$

$$\begin{align*}
\hat{H}_X & = \sum_{ij\sigma} X_{ij\sigma} (\hat{n}_{i\sigma} + \hat{n}_{j\sigma}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}, \\
\hat{H}_Y & = \sum_{ij\sigma} Y_{ij\sigma} \hat{n}_{i\sigma} \hat{n}_{j\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}, \quad (5, 6)
\end{align*}$$

with the constant term depending only on $g$ and the total particle density $n = \hat{n}_\uparrow + \hat{n}_\downarrow$, which is fixed; we mostly consider densities $n \leq 1$ since $|\psi(0)| = 0$ otherwise. Here $T_{ij\sigma}$ is the Fourier transform of $E_{k\sigma} = (1 - 2n_{0\sigma}^k) \hat{E}_{k\sigma}$, and the other parameters are given by

$$h = -\frac{1}{2L} \sum_{k\sigma} (1 - (1 + g^2) n_{0\sigma}^k) \hat{E}_{k\sigma}, \quad (7)$$

$$U = \frac{1 - g^2}{g^2 L} \sum_{k\sigma} (1 - (1 - g^2) n_{0\sigma}^k) \hat{E}_{k\sigma}, \quad (8)$$

$$X_{ij\sigma} = \frac{1}{2g} \left[ (1 - g) T_{ij\sigma} + (1 + g) \tilde{T}_{ij\sigma} \right], \quad (9)$$

$$Y_{ij\sigma} = \frac{1 - g}{2g^2} \left[ (1 + g^2) T_{ij\sigma} + (1 - g^2) \tilde{T}_{ij\sigma} \right], \quad (10)$$

where $\tilde{T}_{ij\sigma}$ is the Fourier transform of $\hat{E}_{k\sigma}$, and $L$ is the number of lattice sites.

A model with arbitrary non-interacting dispersion $\epsilon_k$ can now be obtained as follows. For given band dispersion $E_{k\sigma}$ we construct the Fermi sea via $t_{0\sigma}^k = \Theta(-E_{k\sigma})$ and let $\hat{E}_{k\sigma} = E_{k\sigma} \geq 0$. Then we put $E_{k\sigma} = \epsilon_k - \epsilon_{\text{F}}$, and adjust the Fermi energies $\epsilon_{\text{F}}$ so that the starting wavefunction $|\phi\rangle$ is a Fermi sea with desired densities $n_{\sigma} = \frac{1}{L} \sum_k n_{0\sigma}^k$. In the following we assume $\sum_k \epsilon_k = 0$ for convenience, hence $\epsilon_{\text{F}} \equiv \frac{1}{L} \sum_k \epsilon_k n_{0\sigma}^k \leq 0$.

For each $0 \leq g \leq 1$ the Gutzwiller wavefunction $|\psi(g)\rangle = \hat{K}(g) |\phi\rangle$ is the exact ground state of the extended Hubbard Hamiltonian [4]. It contains the kinetic energy $\hat{H}_t$ of a single band $\epsilon_k$, which is independent of $g$, and an optional Zeeman term $\hat{H}_h$, absent for $\tilde{n}_\uparrow = \tilde{n}_\downarrow$. For $g < 1$, $\hat{H}$ contains interactions that involve at most two sites: a repulsive on-site interaction $\hat{H}_U$ and correlated hopping terms $\hat{H}_X$ and $\hat{H}_Y$, whose amplitudes are related by $g Y_{ij\sigma} = (1 - g)^2 (T_{ij\sigma} + X_{ij\sigma})$. Note that $X_{ij\sigma}$ and $Y_{ij\sigma}$, and $U$ all diverge in the limit $g \to 0$. Similar interaction terms appear in models with superconducting gossamer ground states [2, 3, 4], but here those states cannot be lower in energy than $|\psi(g)|$. Apart from $g$, the magnetic field and the strength and range of the interactions depend on the chosen band dispersion $\epsilon_k$ and the densities $n_\sigma$. To illustrate the behavior of the amplitude $\tilde{T}_{ij\sigma}$ appearing in [9-12] we now discuss several examples.

One-dimensional systems. The dispersion for a one-dimensional ring with nearest-neighbor hopping $-t < 0$ is $\epsilon_k = -2t \cos(k)$. For the Fourier transform of $E_{k\sigma} = \epsilon_k - \epsilon_{\text{F}}$ we find

$$\tilde{T}_{j \pm 1, \sigma} = t \left[ 2n_\sigma - 1 + \frac{1}{\pi} \sin(\pi n_\sigma) \right], \quad (11)$$

$$\tilde{T}_{j + \tau, \sigma} = \frac{4t}{\pi (r^2 - 1)} \left[ r \sin(\pi n_\sigma r) \cos(\pi n_\sigma) \right], \quad (12)$$

which falls off algebraically at large distances. At half-filling ($n_\sigma = 1/2$) it is on the order of $1/r^2$ and alternates in sign for even $r$, while vanishing for odd $r$. This long-range behavior of $\tilde{T}_{ij\sigma}$ is rather generic. As another example we consider $1/r^\alpha$ hopping, $T_{j + \tau, \sigma} = \alpha (1 - 1/|r|)$ with dispersion $\epsilon_k = \frac{\alpha}{r}$, for which the corresponding Hubbard model was solved by Gebhard et al. (see Ref. 7 for a review). We obtain

$$\tilde{T}_{j + \tau, \sigma} = \frac{(-1)^\tau t}{\pi r^{2\alpha}} \left[ 1 - i \pi (2n_\sigma - 1) r - e^{-2\pi i n_\sigma r} \right], \quad (14)$$

again with contributions proportional to $1/r$ (absent for half-filling) and $1/r^2$. Similar power-law behavior is typically found in dimensions $D = 2, 3$.

Infinite-dimensional systems. Nearest-neighbor hopping $t = 1/\sqrt{2D}$ on a hypercubic lattice with dispersion $\epsilon_k = -2t \sum_\alpha \cos k_\alpha$ yields the density of states $\rho_{\text{hc}}(\epsilon) = \exp(-\epsilon^2/2)/\sqrt{2\pi}$ in the limit $D \to \infty$. In order to construct the corresponding amplitude $\tilde{T}_{ij\sigma}$ further assumptions about its symmetry are necessary. Following Ref. 13 we assume that it depends only on the “taxi-cab” distance $||\mathbf{R}|| = \sum_{\alpha = 1}^D |R_\alpha|$ and use the appropriate scaling $\tilde{T}_{ij\sigma} = T_{r, \sigma}/\sqrt{2^{(r^2 - 1)/r}}$ where $r = ||\mathbf{R}_i - \mathbf{R}_j|| \geq 0$. We then obtain

$$\tilde{T}_{r, \sigma} = \int |\epsilon - \epsilon_{\text{F}}| \rho_{\text{hc}}(\epsilon) \frac{H_{\epsilon_{\text{F}}}}{\sqrt{r}} d\epsilon, \quad (15)$$

$$\tilde{T}_{2r, 1, \sigma} = (1 - 2n_\sigma) \delta_{r, 0}, \quad (16)$$

$$\tilde{T}_{2r, 2, \sigma} = 2 \rho_{\text{hc}}(\epsilon_{\text{F}}) \frac{|H_{\epsilon_{\text{F}}}|}{\sqrt{2(r+2)}}. \quad (17)$$
where $H_{0\sigma}(x)$ are Hermite polynomials. At half-filling we find $T_{2\sigma}^* \sim r^{-5/4}$, corresponding to an effective correlated hopping range $\sum_{r} T_{r\sigma}^* 2$ of order unity. For other densities of states $\rho(\epsilon)$, in particular those with finite bandwidth, it is also possible construct a corresponding dispersion $\epsilon_k$ \cite{15}, and then derive $T_{ij\sigma}$ and $T_{ij\sigma}$ in a similar fashion.

**Response to external magnetic field.** Returning to the case of arbitrary dispersion and densities, we note that according to the equation of state \cite{10} the ground-state magnetization $m = \hat{n}_\uparrow - \hat{n}_\downarrow$ is nonzero if an external magnetic field $h$ is present. For the homogeneous susceptibility $\chi$ we obtain
\begin{equation}
\chi(h)^{-1} = \frac{\partial h}{\partial m} = \frac{1}{4} \sum_{\sigma} \frac{1 - (1 - g^2)^2 n_{\sigma}}{\rho(\epsilon_{F\sigma})}. \quad (18)
\end{equation}

In the limit of zero field this reduces to $\chi(0) = \chi_0/[1 - (1 - g^2)^2 n_{\sigma}/2]$. As expected the system behaves like a correlated paramagnet, i.e., the interactions enhance the Pauli susceptibility $\chi_0 = 2\rho(\epsilon_F)$ of the uncorrelated system. However, it should be kept in mind that the interaction parameters \cite{9,10} do not remain constant when the parameters $h$ or $m$ are varied. Fig. 1 shows the magnetization as a function of magnetic field for a one-dimensional ring at half-filling. Interestingly, for nearest-neighbor hopping the upward curvature of these magnetization curves is very similar to Bethe-ansatz results for the pure Hubbard model \cite{19,20,21}, where a metal-insulator transition occurs at $U_c = 0^+$. By contrast, for $1/r$ hopping the magnetization curves are strictly linear, $m = \chi(0)h$, due to the constant density of states.

**Metal-insulator transition.** For an unpolarized half-filled band ($n = 1$, $\epsilon_{F\sigma} = 0$), the ground-state wave function $|\psi(g)\rangle$ describes a metal for $g > 0$ and an insulator for $g = 0$. In the insulating state there are no doubly occupied sites, the discontinuity of $n_{k\sigma}$ at the Fermi surface vanishes, and the kinetic energy $\langle H_I \rangle$ is zero. This Mott metal-insulator transition in the ground state of $\hat{H}$ occurs at infinite interactions \cite{3,4}, in contrast to the variational BR transition, or numerical results for the Hubbard model in infinite dimensions \cite{12}.

Nevertheless we may, somewhat artificially, shift the transition to finite interactions as follows. Clearly $\langle |\psi(g)\rangle \rangle$ remains the ground state when we multiply $\hat{H}$ by a positive $g$-dependent factor, although qualitatively different Hamiltonians may then result in the limit $g \rightarrow 0$. For example, for the Hamiltonian $\hat{H}^{(1)} = g \hat{H}$ the $X$ term has a finite limit, while $\hat{H}^{(2)} = g^2 \hat{H}$ yields a vanishing $X$ term and finite $Y$ and $U$ terms; in both cases the quadratic kinetic energy vanishes at $g = 0$. In particular we may conclude that for any dispersion $\epsilon_k$ the Hamiltonian
\begin{equation}
\hat{H}' = \sum_{i \neq j, \sigma} Y_{ij} \hat{c}_{i\sigma}^\dagger \hat{n}_{j\sigma} \hat{c}_{j\sigma}^\dagger + \hat{U}' \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad (19)
\end{equation}
where $Y_{ij}$ is the Fourier transform of $\epsilon_k(1 - n_{k\sigma}^0)$, has the exact ground state $|\psi(g = 0)\rangle$ at half-filling if $U' \geq U'_c$, with critical interaction $U'_c = -\sum \epsilon_{0\sigma} \approx |\epsilon_0|$. Interestingly, the uncorrelated kinetic energy also sets the energy scale of the BR transition in the Gutzwiller approximation \cite{3}, where $U'_BR = 8|\epsilon_0|$. Although $H'$ is not a standard Hubbard Hamiltonian, it nonetheless appears to be the simplest model with a BR-type transition to an exact insulating ground state at finite Hubbard interaction.

**Ground-state expectation values.** The separate expectation values of the kinetic energy $\langle \hat{H}_I \rangle$ and the interaction terms $\hat{H}_X$, $\hat{H}_Y$, and $\hat{H}_U$ can be calculated from the quantities $n_{k\sigma} = \langle \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} \rangle$, $d = \frac{1}{2} \sum_i \langle \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle$, $x_{ij\sigma} = \langle \hat{n}_{i\sigma} \hat{c}_{j\sigma}^\dagger \hat{c}_{j\sigma}^\dagger \rangle$, and $y_{ij\sigma} = \langle \hat{n}_{i\sigma} \hat{n}_{j\sigma} \hat{c}_{j\sigma}^\dagger \hat{c}_{j\sigma}^\dagger \rangle$. Using the methods of \cite{14,15} it can be shown that for the GWF the
Fourier transforms of the latter are given by

\[ x_{k\sigma} = \delta_{k\sigma}^0 \left[ n_{\bar{\sigma}} - \frac{1 - n_{k\sigma}}{1 - g} \right] - \frac{(1 - n_{k\sigma}) g n_{k\sigma}}{1 - g} - d, \quad (20) \]

\[ y_{k\sigma} = \delta_{k\sigma}^0 \left[ n_{\bar{\sigma}} - \frac{1 - n_{k\sigma}}{(1 - g)^2} \right] + \frac{(1 - n_{k\sigma})^2 n_{k\sigma}}{(1 - g)^2} - d, \quad (21) \]

i.e., only the momentum-space distribution \( n_{k\sigma} \) and the double occupancy \( d \) are needed. They may be evaluated numerically by Monte-Carlo methods, but are also available in closed form under certain circumstances. For one-dimensional systems with symmetric Fermi sea \( (n_{k\sigma} = n_{0-k\sigma}) \) both quantities have been calculated analytically \cite{14, 17}. In dimension \( D = 2, 3 \) high-order perturbative methods can be used \cite{11}. The Gutzwiller approximation \cite{7}, with piecewise constant momentum distribution \( n_{k\sigma} \), is recovered in infinite dimensions \cite{3}.

The expectation values of the various parts of \( \tilde{H} \) are shown in Fig. 2 for nearest-neighbor hopping in \( D = 1 \) and \( D = \infty \) at half-filling. We note that \( \langle \tilde{H}_X \rangle \) approaches a constant for \( g \to 0 \), while \( \langle \tilde{H}_Y \rangle \) and \( \langle \tilde{H}_T \rangle \) diverge. This behavior occurs for all \( D \), since \( d \sim g^2 \ln(1/g) \) in one dimension \cite{14, 17}, \( d = o(g) \) in all finite dimensions \cite{10, 11}, and \( d \sim g \) in infinite dimensions. We may thus conclude that the penalty that \( \tilde{H}_T \) imposes on double occupancies is compensated by assisted hopping due to the nonstandard three-body interaction \( \tilde{H}_Y \).

The effect of correlated hopping is also apparent when comparing to the pure Hubbard ring with \( 1/r \) hopping, which features a metal-insulator transition at \( U_r = 2\pi \) with continuous nonzero double occupancy \( d \). For comparison with previous studies of variational wavefunctions in the vicinity of this transition \cite{10, 17}, \( d \) vs. \( U \) is shown in the inset of Fig. 2. The results for both models with \( 1/r \) hopping agree for weak interactions, but the energy gain from correlated hopping leads to a larger number of doubly occupied sites for strong coupling in the model \cite{4, 21}, as expected.

**Quasiparticle excitations.** The known ground state of \( \tilde{H} \) suggests that it might also be possible to calculate dynamical properties of the model, such as the spectral function. Unfortunately the construction of exact excited states is not straightforward, be it with one added or removed particle, or with charge or spin excitations. We therefore proceed by considering the variational states \cite{2, 21}

\[ |k\sigma\rangle = \hat{K} \hat{b}_{k\sigma}^\dagger \phi = \begin{cases} \hat{K} \hat{c}_{k\sigma}^\dagger \phi & \text{if } n_{k\sigma}^0 = 0 \\ \hat{K} \hat{c}_{k\sigma} \phi & \text{if } n_{k\sigma}^0 = 1 \end{cases}, \quad (22) \]

whose mean energy is

\[ E_{k\sigma}^\pm = \frac{\langle k\sigma | \tilde{H} | k\sigma \rangle}{\langle k\sigma | k\sigma \rangle} = \frac{\langle \phi | \phi \rangle}{\langle k\sigma | k\sigma \rangle} \tilde{E}_{k\sigma}, \quad (23) \]

where the commutator relations \( [\hat{b}_{k\sigma}, \hat{b}_{k'\sigma}^\dagger] = \delta_{kk'} \delta_{\sigma\sigma'} \) and \( [\hat{b}_{k\sigma}, \hat{b}_{k'\sigma'}] = 0 \) were used. The states \( |k\sigma\rangle \) are mutually orthogonal and their energy is thus an upper bound to the quasiparticle energy for momentum \( k \) and spin \( \sigma \).

The variational energy to add a particle (i.e., \( n_{k\sigma}^0 = 0 \)) is

\[ E_{k\sigma}^+ = \frac{g^2 |\epsilon_k - \epsilon_{\sigma\bar{\sigma}}|}{(1 - (1 + g))(1 - g)n_{\sigma} + (1 + g)n_{k\sigma}}, \quad (24) \]

while for the removal of a particle (with \( n_{k\sigma}^0 = 1 \))

\[ E_{k\sigma}^- = \frac{g^2 |\epsilon_k - \epsilon_{\sigma\bar{\sigma}}|}{(1 + g)(1 - (1 + g)n_{\sigma} + (1 + g)n_{k\sigma}) - 1 - 2g}, \quad (25) \]

Clearly the quasiparticle excitations are gapless, since \( E_{k\sigma}^\pm \to 0 \) close to the Fermi surface. Fig. 3 shows these energies for one-dimensional nearest-neighbor hopping at half-filling.

**Conclusion.** We have constructed and characterized a new class of itinerant electron models for which the metallic Gutzwiller wavefunction is an exact ground state, due to the interplay of Hubbard interaction and correlated hopping. For a half-filled band a Mott metal-insulator transition similar to the Brinkman-Rice scenario occurs, illustrating Mott’s original idea of a quantum phase transition entirely due to charge correlations without magnetic ordering. Further study of the elementary excitations in these models should be fruitful.

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