Exact transformation for spin-charge separation of spin-$\frac{1}{2}$

Fermions without constraints

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Abstract

We demonstrate an exact local transformation which maps a purely Fermionic manybody system to a system of spinfull Bosons and spinless Fermions, demonstrating a possible path to a non-Fermi liquid state. We apply this to the half-filled Hubbard model and show how the transformation maps the ordinary spin half Fermionic degrees of freedom exactly and without introducing Hilbert space constraints to a charge-like “quasicharge” fermion and a spin-like “quasispin” Boson while preserving all the symmetries of the model. We present approximate solutions with localized charge which emerge naturally from the Hubbard model in this form. Our results strongly suggest that charge tends to remain localized for large values of the Hubbard $U$. 

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The Hubbard model is a paradigm for one of the most difficult quantum many-body systems; strong interactions competing with the kinetic energy in a dense electron gas. These problems must be explored either analytically by relatively poorly controlled approximate methods or by methods such as Monte-Carlo, dynamical mean field theory (DMFT) or finite size calculations. A major difficulty is the absence of a framework for such systems that competes in simplicity and rigor with conventional Landau Fermi-liquid theory.

A particularly intriguing scenario for non-Fermi liquid behavior is “spin-charge separation” with a low-energy effective theory where spin and charge excitations are decoupled. This idea has attracted widespread attention because it might provide a route to high-temperature superconductivity in a system with strong local repulsion. In 1-D it is known through the use of “bosonization” that spin-charge separation does occur at low energy.\[1\] In higher dimensions, much less is known. The usual approach to spin charge separation is to construct electron operators as composite objects consisting of a charge part, the “holon”, and a spin part, the “spinon”. To avoid unphysical states constraints have to be included which are then treated by approximate methods.\[2\]

Here we shall construct electron operators as composites of charge-like and spin-like operators that do not give rise to any unphysical states and thus avoids introducing any constraints. An exact local mapping which is valid in all dimensions will be shown to exist from a purely Fermionic manybody system to an equivalent system of Fermions and spin-like operators obeying Bosonic commutation relations between different lattice sites. We shall explore this with the 2-D Hubbard model, for which the resulting mapping bears a resemblance to the mappings of the local Hilbert space achieved by introducing spinons and holons.

**Transformation to quasiparticle operators.**

Let \( n_r \) be the particle number at site \( r \), and \( n_\uparrow \) and \( n_\downarrow \) be respectively the number of up and down electrons: \( n_r = n_{\uparrow,r} + n_{\downarrow,r} \). Since the Hubbard interaction obeys \( n_{\downarrow,r} n_{\uparrow,r} = \frac{1}{2} (n_r - 1 + (n_r - 1)^2) \), by choosing the chemical potential appropriately we can replace the usual Hubbard interaction with the particle-hole symmetric interaction \( \frac{1}{2} U (n_r - 1)^2 \). We thus write the Hubbard model in the particle-hole symmetric form \( H = -t \sum_{\langle rr' \rangle} (c_{s,r}^\dagger c_{s,r'} + CC) + U \sum_r \frac{1}{2} (n_r - 1)^2 \) where the sum is over all sites and nearest neighbor bonds counted.
once.

We now demonstrate an exact transformation of the local operator algebra of the Hubbard model to new Fermionic $CP^1$ “quasicharge” $\hat{c}_r$ and $SU(2)$ “quasispin” operators $q^i_r$ that obey, respectively, Fermi and Bose statistics. The operators are given by

$$\hat{c}_r = c^\dagger_{\uparrow,r}(1 - n_{\downarrow,r}) + (-1)^r c^\dagger_{\downarrow,r} n_{\uparrow,r}$$

(1)

$$q^+_r = (c^\dagger_{\uparrow,r} - (-1)^r c^\dagger_{\downarrow,r}) c_{\downarrow,r}$$

(2)

$$q^-_r = (q^+_r)^\dagger$$

$$q^z_r = \frac{1}{2} - n_{\downarrow,r}$$

where $-1^r$ is $\pm 1$ depending on which sublattice site $r$ is on. We define the $x$ and $y$ component of quasispin by

$$q^x_r = \frac{1}{2} (q^+ - q^-)$$

and

$$q^y_r = \frac{1}{2} i (q^+ - q^-).$$

The factor appearing as $(-1)^r$ can in fact be chosen as an arbitrary phase, but is fixed here to preserve symmetries specific to the Hubbard model. This “nonlinear” transformation generalizes earlier work on transformations that were strictly canonical, and hence did not alter commutation relations of the fermi operators.[3, 4]

The new operators obey the following algebra, which can be verified by straightforward manipulations: \{ $\hat{c}_r, c^\dagger_r$ \} $= \delta_{rr'}$ , \{ $c^\dagger_r, q^+_r$ \} $= 0$ , \{ $c^\dagger_r, q^+_r$ \} $= 0$ , \{ $q^+_r, q^+_r$ \} $= i \delta_{rr'} \sum_k \epsilon_{ijk} q^k_r$.

We thus find that $q^i_r, c^\dagger_r$ and $\hat{c}_r$ are respectively independent spin half bosonic and “spinless” Fermionic operators. The usual operators are given by

$$c^\dagger_{\uparrow,r} = \hat{c}_r \left( \frac{1}{2} + q^+_r \right) + (-1)^r \hat{c}^\dagger_{\downarrow,r} \left( \frac{1}{2} - q^z_r \right)$$

(3)

$$c^\dagger_{\downarrow,r} = q^- \left( \hat{c}_r - (-1)^r \hat{c}^\dagger_{\uparrow,r} \right).$$

We define the quasicharge operator as $n^\ell_r = \hat{c}^\dagger_{\ell,r} \hat{c}_r$. We find the following relations with the usual operators expressed in terms of ordinary Fermions: $n_r = 1 - 2 n^\ell_r q^+_r$, $s^i_r = (1 - n^\ell_r) q^i_r$ and $n^\ell_r = (n_r - 1)^2$ where $s^i_r = \frac{1}{2} \sum_{\alpha,\beta} c^\dagger_{\alpha,r} \sigma^i_{\alpha,\beta} c^\dagger_{\beta,r}$, with $\sigma^i$ the Pauli matrices. We also define the local ”pseudospin” operators $p^i_r = n^\ell_r q^i_r$ which are the generators of the $SU(2)$ algebra which corresonds to ”rotations” between the empty and doubly occupied states.[5]

The formal resemblance to spin symmetry has led to the name pseudospin. The total $z$-component of pseudospin can therefore be seen to be half the number of doubly occupied sites minus the number of empty sites, which is precisely the charge relative to half filling. Pseudospin is a symmetry of the particle-hole symmetric Hubbard model but is broken by a chemical potential.
We note that, aside from phase factors, the quasicharge operators always create even charged states from odd and vice versa, as they must since they are Fermionic. However, there is a precise phase relationship which is not so easily interpreted that is enforced by the commutation relations and symmetries.

Our Hubbard model can now be rewritten exactly in terms of the quasiparticle operators as

\[ H = t (T_0 + T_1 + T_{-1}) + U h_U \]  

with \( h_U = \frac{i}{2} \sum_r \hat{c}_r^\dagger \hat{c}_r \) and

\[ T_0 = \frac{1}{2} \sum_{\langle r, r' \rangle} (1 + 4 \mathbf{q}_r \cdot \mathbf{q}_{r'}) (\hat{c}_r^\dagger \hat{c}_{r'} + CC) \]

\[ T_1 = \frac{1}{2} \sum_{\langle r, r' \rangle} -1^r (1 - 4 \mathbf{q}_r \cdot \mathbf{q}_{r'}) (\hat{c}_r^\dagger \hat{c}_{r'}^\dagger) \]

and \( T_{-1} = T_1^\dagger \). In this representation, the symmetry under the entire SU(2) quasispin rotation is manifest and we note that the Hubbard interaction becomes simply the quasicharge number operator.

We define total quasipin \( Q \), spin \( S \) and pseudospin \( P \) respectively by \( Q = \sum_r \mathbf{q}_r \) etc. \( P, Q \) and \( S \) all obey the SU(2) algebra \([ P_i, P_j ] = i \sum_k \epsilon_{ijk} P_k \) etc. We see from the definitions above Eq. [4] the relationship, \( p_r^i = n_r^i q_r^i \) and \( s_r^i = (1 - n_r^i) q_r^i \). Thus \( Q = P + S \), i.e. quasipin can be exactly split into pseudospin and spin, with \( n_r^i \) and \( (1 - n_r^i) \) providing the projection operator of \( Q \) into either spin or pseudospin. Since \( Q \) commutes with \( \hat{c}_r^\dagger \) and the Hubbard Hamiltonian \( H \) depends on \( \mathbf{q}_r \) only through rotationally invariant terms, we conclude that \([ H, Q ] = 0 \). We further know that the Hubbard model commutes with ordinary spin whereby \([ H, S ] = 0 \). We can therefore conclude that \([ H, P ] = 0 \), which confirms the well known invariance under pseudospin rotations.

The operators \( T_{\pm 1,0} \) are identical to the operators defined in Ref. [7] and used in a perturbation expansion in \( t/U \). It is clear from their definitions that \( T_{\pm 1} \) couples different Hubbard bands defined by the sectors given by different values of \( \langle h_U \rangle \) whereas \( T_0 \) does not. We observe \([ T_{0, \pm 1}, Q ] = 0 \). It can be inferred that \([ T_{0, \pm 1}, P ] = 0 \) since \( T_{0, \pm 1} \) is known to commute with ordinary spin.

We now define the usual canonical transformation \( S \) which splits the Hamiltonian into pieces that preserve total quasipin. We define \( S = i(T_{-1} - T_1) + i [ T_0, (T_1 + T_{-1}) ] \)
and it straightforward to show that $[\mathcal{S}, h_U] = (T_{-1} + T_1)$, whereby it follows that $H_{\text{eff}} = e^{it\mathcal{S}/U} H_{\text{hub}} e^{-it\mathcal{S}/U} = H_{\text{hub}} + i t [\mathcal{S}, H_{\text{hub}}] / (2U^2) + t^2 [\mathcal{S}, [\mathcal{S}, H_{\text{hub}}]] / (2U^2)^2 + \ldots \equiv H_{q\hat{c}} + H_q + O(t^3 / U^2)$ splits into two terms. The first term $H_q$ is the ordinary spin interaction in the “spin-only” sector

$$H_q = J \sum_{\langle rr' \rangle} (q_r q_{r'} - \frac{1}{4})$$

where $J = 4t^2 / U$ and the second term $H_{q\hat{c}}$ couples quasispin and quasicharge

$$H_{q\hat{c}} = \sum_{\langle rr' \rangle} (U h_U + t T_0 + \frac{t^2}{4U} (n_r^f + n_{r'}^f) (q_r q_{r'} - \frac{1}{4})) +$$

$$+ \frac{t^2}{4U} \sum_{\langle rr' r'' \rangle} \left( c_{r''}^\dagger c_{r''} + c_{r''}^\dagger \hat{c}_r \right) (1 - q_r q_{r'} + q_r q_{r''} - q_{r'} q_{r''} + i q_r \cdot (q_{r'} \times q_{r''})) .$$

The last summation runs over all three-site neighbors connected by links. Terms of order $t^2 / U$ which are already present to order $t$ or $U$ are ignored. According to the results of Ref. [7], to all orders in $t / U$ the operator $\mathcal{S}$ which diagonalizes total quasicharge is a polynomial of $T_{0, \pm 1}$, and hence to all orders in perturbation theory, the transformation by $e^{it\mathcal{S}/U}$ will preserve all the symmetries $Q$ and $P$ in this formulation.

The spin-only sector

Under this canonical transformation the eigenstates of $H_{\text{eff}}$ will map to the eigenstates of the Hubbard model represented by the bare quasiparticle operators through the transformation $e^{it\mathcal{S}/U}$. We let $|\Psi_{\text{eff}}\rangle$ be eigenstates of $H_{\text{eff}}$ and $|\Psi\rangle = e^{it\mathcal{S}/U} |\Psi_{\text{eff}}\rangle$. Adapting Ref. [7] to our problem, there will be a “zeroth Hubbard band” or “spin-only sector” of solutions corresponding to $n_r^f |\Psi_{\text{eff}}\rangle$ being identically zero so that $H_{\text{eff}}$ reduces exactly to $H_q$. We conclude $\langle H_{q\hat{c}} \rangle_{\Psi_{\text{eff}}} \equiv 0$ is identically zero and the effective Hamiltonian of the zeroth subband to order $t^2 / U$ is exactly the Heisenberg model.

What can we conclude from symmetries about the properties of the zeroth Hubbard band? It must be remembered that $N_{\text{tot}}^f = \sum_r n_r^f$ is not a “good quantum number” i.e. is neither invariant under the symmetries nor under $e^{it\mathcal{S}}$. We have therefore no information about $\langle n_r^f \rangle_\Psi$ from symmetry arguments alone. However, we see that $n_r^f |\Psi_{\text{eff}}\rangle = 0$ throughout the entire lattice in the entire zeroth Hubbard subband. We can therefore conclude that
\[ \langle P \rangle_{\Psi} = 0. \] Since \( P \) commutes with \( S \), this assertion survives to all orders in perturbation theory and we can conclude that \( \langle P \rangle_{\Psi} = 0 \). In fact quasispin and ordinary spin coincide. Since \( \langle n \rangle = \langle 1 - 2P_z \rangle \) is equal to physical charge, we see that the spin-only sector has indeed charge density corresponding to half filling.

**Extended states in the charge-only sector**

The pseudospin is given by \( P^2 = \sum_{r,r'} q_r \cdot q_{r'} n^f_r n^f_{r'} \). If there is exactly one quasicharge, we conclude from the fact that \( q^2_r = 3/4 \) that \( \langle P^2 \rangle = 3/4 \). We have thus identified the lowest nonzero quasicharge sector with the spin half representation of pseudospin, exactly what we need to associate it with one added positive or negative physical charge.

We can derive a set of extended charge states in the dilute limit by a mean field treatment of Eq. 7, replacing \( q_r \cdot q_{r'} = \langle q_r \cdot q_{r'} \rangle_{H_q} \). In two dimensions, these have the spectrum

\[
E_k = \frac{1}{2} U - 4t\alpha(\cos k_x + \cos k_y) + \frac{t^2}{4U}((\cos 2k_x + \cos 2k_y)(1 - e_2) + 2 \cos k_x \cos k_y(1 - e_{\sqrt{2}}))
\]

where \( \alpha = |(1/4 + e_1)| \) and where \( e_1 = \langle q_r q_{r'} \rangle \), \( e_{\sqrt{2}} \) and \( e_2 \) denote nearest neighbor and longer range Heisenberg correlations. Using the numerical value \( e_1 = -0.33972(2) \) we find \( \alpha = 0.08972 \). We find a quasicharge spectrum bounded by \( U/2 \pm 8\alpha t + O(t^2/U) \) and shown in the shaded region of Fig. 2.

**The Nagaoka instability and localized states**

The present calculation makes the “Nagaoka theorem” natural. Consider Eq. 4 in the case where the quasispins are perfectly aligned along the quasispin z axis. In this case \( q_r \cdot q_{r'} = \frac{1}{4} \), the operator \( T_{\pm 1} \) will be identically zero and the kinetic energy \( T_0 \) becomes precisely \[ \sum_{r,r'} \hat{c}^\dagger_r \hat{c}_{r'} + \hat{c}^\dagger_{r'} \hat{c}_r. \] These are quasicharges moving independently of the ferromagnetic quasispins and are ordinary holes in a perfect 2-D ferromagnet which the kinetic energy \[-2t(\cos k_x a + \cos k_y a) + \frac{1}{2} U \] in the thermodynamic limit.

The Nagaoka theorem states that as \( U \to \infty \) a single charge causes the ground state of \( H \) to become ferromagnetic. This Nagaoka ferromagnet with charge one has Hubbard
The two smallest quasiferromagnetic clusters is shown. The shaded regions include the sites on which charge is approximately confined.

Energy $E_{\text{ferro}} = \frac{1}{2} U - 4t$, whereas the antiferromagnetic solution with a single quasicharge has energy $E_{\text{antiferro}} = 2\Omega J (e_1 - \frac{1}{4}) + U/2 - 8\alpha t$ where $\Omega$ is the number of lattice sites in the system. We therefore find that $E_{\text{ferro}} < E_{\text{antiferro}}$ when the inequality $U > \Omega t (1 + 2\alpha)/(1 - 2\alpha)$ holds. We see that whether or not there is Nagaoka ferromagnetism depends on which order we take $U$ and $\Omega$ to infinity.

The argument can be used to estimate when the antiferromagnet becomes unstable to ferromagnetic ordering. (See also Ref. [9]). Let us consider a quasicharge density of $\rho < 1$. We see that if $\rho$ obeys $\rho < t/U (1 + 2\alpha)/(1 - 2\alpha)$ the dilute ferromagnet will be energetically favored over a collection of extended quasicharge states, essentially reproducing the argument by Ioffe and Larkin.

Using the previous ideas, we shall study localized states in a 2-D antiferromagnet. As we have seen, a quasicharge hops freely on a ferromagnetic bond where $q_r \cdot q_{r'} = \frac{1}{4}$. In a mean field treatment of the quasispins, to linear order in $t$ a quasicharge cannot hop an a bond with antialigned quasispins since $\langle q_r \cdot q_{r'} \rangle = -\frac{1}{4}$.

Starting with a patch of locally Neel ordered quasispins oriented along $\pm q^z$ we consider a quasispin state with nearby spins flipped relative to the Neel state on diagonally adjacent sites of the spin-down sublattice. We note that in the presence of a quasispin ferromagnet oriented along $+z$, quasicharge corresponds to physical charge measured from half filling.

The core of the region will thus be a ferromagnet surrounded by a closed boundary of antialigned spins. Outside this patch, quasispins are allowed to relax, so that far away the system will be a Heisenberg antiferromagnet. The two smallest such configurations are shown in Fig. [1].
We identify the quasispin of the state by constructing the Neel state with the same rotational symmetry around the cluster. The smallest cluster (Fig. 1a) has one flipped spin thus has $Q = \frac{1}{2}$ whereas the cluster with two flipped spins (Fig. 1b) has $Q = 2$. We now add $n_f$ quasicharges to the cluster. According to the definition of pseudospin, in the case where quasicharge is confined to a quasiferromagnetic region with $\mathbf{q}_r \cdot \mathbf{q}_{r'} = \frac{1}{4} + \frac{1}{2} \delta_{rr'}$, it can be shown that $\mathbf{P}^2 = \frac{n_f}{2} \left( \frac{n_f}{2} + 1 \right)$. A cluster with $n_f$ units of quasicharge will thus have pseudospin $P = \frac{1}{2} n_f$ and, from the identity $Q = S + P$, physical spin $S = |Q - \frac{1}{2} n_f|$. The clusters with no quasicharge have pseudospin zero and physical spin equal to quasispin, whereas the charge one cluster will have pseudospin $P = \frac{1}{2}$ and spin $S = Q - \frac{1}{2}$.

The energies of these states are approximate but the spin and pseudospin quantum numbers are exact. As quasicharge is added in the cluster, quasispin, spin and pseudospin continue to be good quantum numbers. Since quasispin is conserved upon adding quasicharge each such configuration has a well defined value of quasispin independent of physical spin or charge and can be calculated in the effective theory. Quasicharge, however, is not a good quantum number, and will change upon transforming back the physical state with $e^{\mu S / U}$.

We estimate the energy by keeping only the part of the kinetic energy linear in $t$ and ignore the spin exchange energy beyond the antiferromagnetic boundary of the cluster. For the smallest $Q = \frac{1}{2}$ cluster we see sixteen bonds that are strongly affected by the localized charge. Four bonds are ferromagnetic with zero energy and twelve bonds are antiferromagnetic with energy $J \times (-\frac{1}{2})$, i.e. they retain about 85% of the energy of the unaffected Neel state $J \times (e_1 - \frac{1}{4}) \approx -0.59 J$.

The energy of these states is compactly written with the spectroscopic-like notation $Q E_S^c$ where $Q$ is the quasispin, $c = 2P^z$ is the charge relative to half filling and $S$ is the spin. Thus $\frac{3}{2} E_0^0$ is the energy of the the smallest uncharged cluster measured with respect to the Heisenberg ground state. We find $\frac{3}{2} E_0^0 = J(12 \times (-\frac{1}{2}) + 16 \times |e_1 + \frac{1}{4}|) \approx 13.74 t^2 / U$. The five kinetic energy eigenvalues of this cluster are $t(-2, 0, 0, 0, 2)$. We thus find $\frac{3}{2} E_0^1 = U / 2 + \frac{3}{2} E_0^0 - 2t \approx U / 2 + 13.74 t^2 / U - 2t$. For the $Q = 2$ cluster we find a kinetic energy for a single charge $-\sqrt{6} t$; there are 16 antiferromagnetic bonds and 8 ferromagnetic bonds giving $2 E_1^1 = U / 2 + 2 E_0^0 - \sqrt{6} t \approx U / 2 + 24.61 t^2 / U - 2.45 t$. The energy of these states are plotted in Fig. 2 and compared to the energy of the band of extended states from Eq. 8. We find that for large $U$ the clusters with localized charge are energetically favored over the extended states. As $U$ becomes larger, larger clusters lower the energy in accordance.
FIG. 2: Energy of the extended and the two simplest localized single-charge states.

with the Nagaoka theorem.

Conclusions

We have demonstrated an exact local mapping from a Fermionic many-body system to system of interacting Bosons and Fermions that does not introduce constraints. The mapping provides a paradigm for a non-Fermi liquid behavior for correlated Fermions valid in any dimension. Applied to the 2-D Hubbard model the transformation makes precise earlier attempts that relied on approximations and constraints to discuss spin and charge as composite operators. Our calculations supports the idea of low energy localized states where spin is bound to charge in the limit of large $U$.

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