New Mapping for Particles on Lattices with Hard-Core Interactions

Daniel C. Mattis
Department of Physics, University of Utah, Salt Lake City, Utah 84112
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A novel mapping between Hilbert spaces of unequal dimensionalities yields many-body states which exactly satisfy the no-double-occupancy constraints for particles on lattices in arbitrary spatial dimensions. After proving the states are complete, we apply them to Nagaoka's theorem and the *t-J* model. Modifications are suggested suitable for spin-$\frac{1}{2}$ Heisenberg or *X-Y* models and for hard-core bosons. Extensions to "soft-core" potentials such as the Hubbard model, or spin problems for spins $>\frac{1}{2}$, are also indicated.

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The no-double-occupancy rule, equivalent to the hard-core interaction for particles hopping on a lattice, has proved difficult to enforce in dimensions $D > 1$ for SU(2) fermions. The present theory shows how to do so exactly, using a set of "phantom" fermions subject only to the usual anticommutation relations. We map the physical Hilbert space onto a target Hilbert space of larger dimensionality and solve the eigenvalue problem in the target phantom space. This transparent—not to say obvious—procedure should prove useful in many applications. We discuss Nagaoka's ferromagnetism [1] and the *t-J* model as specific examples. With slight modifications the mapping is extended to spin problems such as the *X-Y* and Heisenberg models, to hard-core bosons, and to models with "soft-core" potentials (including the Heisenberg model for spins $1, \frac{3}{2}, \ldots$ and Hubbard's model with finite U) also insoluble in $D > 1$. Aside from these examples the present paper exhibits the key ideas and proof of a "completeness" theorem.

The t-J model.—As the prototype physical problem addressed by our method we first examine hard-core fermions on a lattice. The Hamiltonian H_0 describes hopping on the N vertices of a lattice in D dimensions, by fermions constrained only by mutual repulsion. Augmenting H_0 by nearest-neighbor interactions $J(\vec{\sigma}_i \cdot \vec{\sigma}_j - \hat{n}_i \hat{n}_j)$ (where $\vec{\sigma}_i$ and $\hat{n}_i$ are, respectively, the Pauli and the occupation number operators at the ith site) turns it into the *t-J* model.

Given in terms of "physical" annihilation and creation operators $c_{i,\sigma}$ and $c_{i,\sigma}^\dagger$,

$$H_0 = -t \sum_{(i,j)} \sum_{\sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.}), \tag{1}$$

with sums over all distinct nearest-neighbor bonds (i,j) and spin labels $\sigma = \pm\frac{1}{2}$ (also written as $\uparrow$ or $\downarrow$). The states which constitute the Hilbert space in which (1) operates carry a subscript c. Each is subject to N holonomic constraints,

$$c_{i,\uparrow} c_{i,\downarrow} |\psi\rangle_c = 0. \tag{2}$$

As a consequence, this Hilbert space is spanned by 3^N rather than 4^N distinct states. The number of electrons which can be accommodated is necessarily $\leq N$. For N electrons there must be 1 electron per site. There are 2^N such states, all degenerate with zero energy, for which no charge fluctuations or transport are allowed. When $J = 0$, Nagaoka [1] showed that the introduction of a single hole ($N \to N - 1$) lifts much of this degeneracy on a bipartite lattice, for $D > 1$. The resulting ground state for one hole is ferromagnetic with multiplicity (degeneracy) $2N$. Ever since Nagaoka discovered this result there has been ongoing interest [2] in determining the number υN of holes at which there is a crossover from ferromagnetism to paramagnetism, to fix the "critical" value υ_0 of the hole filling fraction

$$\upsilon = 1 - {}_c\langle \psi | \frac{1}{N} \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} |\psi\rangle_c, \tag{3}$$

for which the $S = 0$ ground state lies lowest, given the lattice geometry in $D > 1$ dimensions. The ferromagnetic configuration is trivially the same as that of free fermions, since the Pauli principle automatically prevents double occupancy by electrons of parallel spin. Thus its energy is easily computed. Calculating the energy of the paramagnetic states is another matter [2]. Below, we present some formulas which are helpful in this regard.

The *t-J* model is of course also subject to the constraints (2). For $\upsilon \to 0$ it coincides with the Heisenberg antiferromagnetic which is known to have a singlet ground state. To $O(J)$ the ground-state degeneracy in Nagaoka's model is thereby lifted completely. But with increasing hole filling factor the *t-J* model proves increasingly difficult to analyze by standard methods. At this date reliable information comes principally from numerical investigations on finite clusters [3]. Our method speaks to this model as well.

Our procedure creates appropriate trial functions in an enlarged space. If desired, these functions can always be projected back onto the physical space [as shown in Eq. (5) below], but generally this should not prove necessary. For

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fermions we propose

$$|\Psi) \equiv \Omega|0\rangle_c \otimes |\phi\rangle_d \quad \text{where } \Omega = \prod_i \Omega_i\,,$$
$$\text{each } \Omega_i \equiv \left(1 + \sum_\sigma \beta_{i,\sigma} c^\dagger_{i,\sigma} d_{i,\sigma}\right)\left(1 + \sum_\sigma \beta^2_{i,\sigma}\tilde{n}_{i,\sigma}\right)^{-1/2},$$
$$\text{and } \tilde{n}_{i,\sigma} \equiv d^\dagger_{i,\sigma} d_{i,\sigma}\,. \tag{4}$$

The auxiliary d's are the phantom operators, a complete set of anticommuting fermions operating in phantom space (labeled by subscript d). The $\beta_{i,\sigma}$ parameters are real [4] and $\neq 0$. For practical purposes we shall eventually take the $\beta_{i,\sigma}$ to be translationally and rotationally invariant, i.e., constant, and arbitrarily large. For present purposes it is good to keep them as individual parameters. The Ω_i factors which make up the operator Ω can be placed in any sequence as the fermion operators are paired, and therefore they commute. From right to left the kets in (4) consist of any normalized (but otherwise arbitrary) state $|\phi\rangle_d$ of the d's, and the "physical" vacuum. The square root terms ensure $|\Psi)$ is normalized. In this transformation, the c operators are annihilated, then transmuted into d phantom operators. Regardless of the choice of parameters, each $|\Psi)$ *always* satisfies the N constraints in Eq. (2) *by inspection.* We next discuss the properties of these states and the uses to which they can be put, first showing that they are a complete set and hence adequate to any task.

States (4) are in fact *overcomplete* as we now see by construction. In $|\Psi)$ let $|\phi\rangle_d$ be selected among d states of the type $|\rho\rangle_d \equiv \prod_{i\subset R_\uparrow} d^\dagger_{i,\uparrow}\prod_{j\subset R_\downarrow} d^\dagger_{j,\downarrow}|0\rangle_d$ in which $R_\uparrow$ is one among all possible subsets of the lattice sites and $R_\downarrow$ a second such subset, possibly overlapping the first. We construct *one* distinct state of the physical operators $|\psi\rangle_c$ for *each* of the 3^N states $|\rho\rangle_d$ in which $R_\uparrow$ and $R_\downarrow$ are *nonoverlapping,* by means of the projection ${}_d\langle 0|\Psi)$:

$$|\psi\rangle_c \equiv C^{-1/2}{}_d\langle 0|\Omega|0\rangle_c \otimes |\rho\rangle_d\,. \tag{5}$$

If $R_\uparrow$ and $R_\downarrow$ do not overlap, the norm is $C = \prod_{i\subset R_\uparrow}\gamma^2_{i,\uparrow}\prod_{j\subset R_\downarrow}\gamma^2_{j,\downarrow}\neq 0$, where $\gamma_{i,\sigma}\equiv\beta_{i,\sigma}/\sqrt{1+\beta^2_{i,\sigma}}$. If the sets $R_\uparrow$ and $R_\downarrow$ share one or more sites, the norm vanishes identically and the corresponding state does not exist. Thus (5) maps the 4^N states of the phantom operators onto all 3^N linearly independent states of the physical particles. Given any Hamiltonian H subject to the hard-core constraints (2) in physical space, one can always construct an equivalent Hamiltonian in the phantom space by choosing the set of $\beta_{i,\sigma}$ appropriately and performing some kind of projection, such as in (5). Although the specific choice we make now is not unique and might not even be optimal, it *does* keep the new Hamiltonian explicitly Hermitian:

$$H_{\text{equiv}} = {}_c\langle 0|\Omega^\dagger H\Omega|0\rangle_c\,. \tag{6}$$

Its eigenstates $|\phi\rangle_d$ will not be a single configuration $|\rho\rangle_d$ but a linear combination of them. We are particularly interested in the ground state of the equivalent Hamiltonian in a specific sector [5] or a variational approximation thereto. Because $|\phi\rangle_d$ inserted in $|\Psi)$ yields a variational solution of the original H in any given sector, the Rayleigh-Ritz principle guarantees that its energy eigenvalue is an upper bound to, or identical to, the ground-state energy of the original H in that same sector. So by comparing the ground states of H_{equiv} for different values of the hole filling fraction we can in principle determine the point at which the crossover from ferromagnetism to paramagnetism occurs in Nagaoka's model. We shall shortly discuss identification of each sector. But first, for the hopping Hamiltonian in Eq. (1) the projection in (6) yields

$$H_{0,\text{equiv}} = -t\sum_{(i,j)}\sum_\sigma \gamma_{i,\sigma}\gamma_{j,\sigma}(d^\dagger_{i,\sigma}d_{j,\sigma} + \text{H.c.}) \times (1-\xi_{i,\sigma}\tilde{n}_{i,-\sigma})(1-\xi_{j,\sigma}\tilde{n}_{j,-\sigma}), \tag{7a}$$
$$\text{where } \xi_{i,\sigma} = 1-\left(\frac{1+\beta^2_{i,\sigma}}{(1+\beta^2_{i,-\sigma})(1+\sum_\sigma\beta^2_{i,-\sigma})}\right)^{1/2}.$$

Upon optimizing the ground-state energy for small clusters where the calculations can be done exactly, we find that the *optimum* $B_{i,\sigma}$ satisfy $\beta_{i,\uparrow}\equiv\beta_{i,\downarrow}\to\infty$. In this limit, the above simplifies to

$$H_{0,\text{equiv}} = -\,t\sum_{(i,j)}\sum_\sigma(d^\dagger_{i,\sigma}d_{j,\sigma} + \text{H.c.}) \times (1-\tilde{n}_{i,-\sigma})(1-\tilde{n}_{j,-\sigma})\,. \tag{7b}$$

As noted earlier, d operators satisfy the usual anticommutation relations and are otherwise under no constraints. $H_{0,\text{equiv}}$ has the appearance of the original hopping operator H_0 as modified by Gutzwiller's projection operator [6]. However, this last appears here not as the inspired *ad hoc* attempt to limit double occupancy it was originally, but as a mathematical consequence of the mapping.

The analysis must include the constants of the motion. Define the local occupation number $n_{i,\sigma} = {}_d\langle\phi|\tilde{n}_{i,\sigma}|\phi\rangle_d$, not necessarily equal to the corresponding value of the physical particles. The hole filling fraction simplifies in the $\beta\to\infty$ limit, and is

$$v_{\text{lim}} = \frac{1}{N}\sum_i\{1 - n_{i,\uparrow} - n_{i,\downarrow} + {}_d\langle\phi|\tilde{n}_{i,\uparrow}\tilde{n}_{i,\downarrow}|\phi\rangle_d\}\,. \tag{8}$$

Note the on-site correlation term here, which is absent in standard treatments in the physical space (where double occupancy is prohibited in principle). Similarly, the average spin projection on the z axis, per site, is

$$S_z/N_{\text{lim}} = \frac{1}{2N}\sum_i\{n_{i,\uparrow} - n_{i,\downarrow}\}\,. \tag{9}$$

A final charge-conjugation transformation proves most useful in the challenging range of parameters where v is still small but metallic behavior has set in:

$$\overline{H}_0 = t\sum_{(i,j)}\sum_{\sigma}(d^\dagger_{i,\sigma}d_{j,\sigma} + \text{H.c.})\tilde{n}_{i,-\sigma}\tilde{n}_{j,-\sigma}\,. \tag{10}$$

The d operators and $\tilde{n}_{i,\sigma}$ now refer to *holes* in otherwise filled bands on the phantom lattice. We use a superposed bar to distinguish the Hamiltonian and the other constants of the motion in the phantom hole representation such as the *physical* hole filling fraction v and magnetization, which assume the form

$$\begin{aligned}\overline{v} &= \frac{1}{N}\sum_i\{{}_d\langle\phi|\tilde{n}_{i,\uparrow}\tilde{n}_{i,\downarrow}|\phi\rangle_d\},\\ \overline{S}_z/N &= \frac{1}{2N}\sum_i\{n_{i,\downarrow} - n_{i,\uparrow}\}.\end{aligned} \tag{11}$$

This latest expression for v is truly novel, although on further examination it seems inevitable. Phantom holes contribute to the number of physical holes *only* to the extent that the phantom holes are *paired.* The Hamiltonian (10) is no less remarkable. Holes of spin σ propagate freely but *only* between nearest-neighbor sites occupied by holes of opposite spin. To achieve Nagaoka's maximally ferromagnetic state for vN physical holes, populate *every* lattice site by a phantom $\downarrow$ hole particle and introduce additional $vN\uparrow$ holes on the lattice. The latter then propagate freely and their total energy $E_{\text{ferro}} = -tNf(v)$ where $f(v)$ can be computed exactly. To estimate the singlet ground-state energy [7], we divide the lattice into $N/2$ dimers, each in a singlet-state configuration: $(1/\sqrt{2})\,(d^\dagger_{1,\uparrow}d^\dagger_{2,\downarrow} + d^\dagger_{2,\uparrow}d^\dagger_{1,\downarrow})\,|0)$. In Nv cells we now add an extra phantom hole, half of spin $\uparrow$ and half $\downarrow$, e.g., $(1/\sqrt{2})d^\dagger_{1,\uparrow}(d^\dagger_{2,\downarrow} \pm d^\dagger_{1,\downarrow})d^\dagger_{2,\uparrow}\,|0)$ having energy $\pm t$. With the aid of Eq. (10) one can obtain the energy of propagation of these compound spin-$\frac{1}{2}$ entities and find that in the sq lattice with $v = \frac{1}{2}$ the total energy of this variational singlet lies somewhat below that of the ferromagnetic ground state. This agrees with the corresponding estimate of 0.49 by Shastry, Krishnamurty, and Anderson [2] based on a different approach. Details will be given elsewhere.

Next we include the exchange interaction H' in the *t-J* model, $J > 0$. In physical space,

$$H' = -\frac{J}{2}\sum_{(i,j)}(c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow} - c^\dagger_{i,\downarrow}c^\dagger_{j,\uparrow})\,(c_{j,\downarrow}c_{i,\uparrow} - c_{j,\uparrow}c_{i,\downarrow})\,. \tag{12}$$

After some algebra the equivalent interaction Hamiltonian for $\beta_{i,\uparrow} \equiv \beta_{i,\downarrow} \to \infty$ is found to be

$$\overline{H}' = -\frac{J}{2}\sum_{(i,j)}\bigg\{\frac{1}{4}[(1-\tilde{n}_{i,\uparrow})\,(1-\tilde{n}_{j,\downarrow})\times(1+\tilde{n}_{i,\downarrow})\,(1+\tilde{n}_{j,\uparrow}) + \text{same } (i\leftrightarrow j)] + [(d^\dagger_{i,\uparrow}d^\dagger_{j,\downarrow}d_{i,\downarrow}d_{j,\uparrow} + \text{same } (i\leftrightarrow j)]\bigg\}. \tag{13}$$

Nagaoka's states of maximal ferromagnetism are explicitly eigenstates of (13) with zero eignevalue. Therefore they can only be stable in a small region near $J = 0$ and $v = 0$. Outside that region the paramagnetic (possibly superconductive) ground state of the *t-J* model [3] will be found among those states possessing equal $\uparrow$ and $\downarrow$ phantom hole populations.

Spins and bosons.—The spin-$\frac{1}{2}$ *X-Y* model is the prototype of bosons hopping on a lattice subject to a hard-core zero-range repulsion [8]. The Heisenberg model augments it by $J_z\sigma_{i,z}\sigma_{j,z}$ type interactions. In the case of the spin Heisenberg ferromagnet the ground-state and one-magnon states are known exactly in all D [9]. One desires to find the multimagnon states. A normalized transformation, suitable for both, could take the now familiar form $|\Psi) = \prod_i(1 + \beta_i\sigma^\dagger_i d_i)\,(1 + \beta_i^2 d^\dagger_i d_i)^{-1/2}\,|\text{all}\downarrow\rangle_\sigma \otimes |\phi\rangle_d$ in which *boson* d's replace spin operators. The initial Hilbert space of dimensionality 2^N is mapped onto an ∞-dimensional harmonic-oscillator target space. The equivalent Hamiltonian which yields the exact ferromagnetic ground state and exact one-magnon states has all $\beta_i \equiv 1$. It is

$$\begin{aligned}H_{\text{equiv}} = &-\frac{J_x}{2}\sum_{(i,j)}(1 + d^\dagger_j d_j)^{-1/2}\,(1 + d^\dagger_i d_i)^{-1/2}\\ &\times(d^\dagger_i d_j + \text{H.c.})\,(1 + d^\dagger_i d_i)^{-1/2}\,(1 + d^\dagger_j d_j)^{-1/2}\\ &-\frac{1}{4}J_z\sum_{(i,j)}\frac{(d^\dagger_i d_i - 1)\,(d^\dagger_j d_j - 1)}{(1 + d^\dagger_i d_i)\,(1 + d^\dagger_j d_j)}\,.\end{aligned} \tag{14}$$

The magnetization has an equally simple form in the phantom space. The quasiparticles carry spin $\frac{1}{2}$. With two of them one can construct 3 elementary excitations of spin 1 (magnons) and 1 of spin 0. Of course, this map is not the only possible choice. If we use $|\Psi)_{\text{HP}} = \prod_i\{\sqrt{1 - d^\dagger_i d_i} + \sigma^\dagger_i d_i\}\,|\text{all}\downarrow\rangle_\sigma \otimes |\phi\rangle_d$ instead, the result is the *XXZ* model in Holstein-Primakoff form [9], which fails if at any site there are ≥ 2 particles. Although the very form of $|\Psi)_{\text{HP}}$ reflects this failure, it *could* be fixed up. But this is not necessary, as Eq. (14) is not subject to any such restrictions and can be used safely to estimate the energy and other properties of multimagnon states.

Soft core.—As our last example we turn to the Hubbard model for fermions with finite zero-range interactions U

[6,10]. At finite U there is finite probability amplitude for double occupancy at each site and the initial and target spaces have the same dimensionality. Still, the method can be applied, e.g.,

$$|\Psi) \equiv \prod_i \left\{ \left(1 + \sum_\sigma \beta_{i,\sigma} c^\dagger_{i,\sigma} d_{i,\sigma} + \lambda_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} \right) \times \left(1 + \lambda_i^2 d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} + \sum_\sigma \beta^2_{i,\sigma} d^\dagger_{i,\sigma} d_{i,\sigma} \right)^{-1/2} \right\} |0\rangle_c \otimes |\phi\rangle_d \ , \quad (15)$$

with $\lambda \propto 1/U^{1/2}$ at large U. Because the $d^\dagger_{i,\sigma} d_{i,\sigma}$ are idempotent expressions such as $(\cdots)^{-1/2}$ are quite easily rationalized. The resulting transformed Hubbard Hamiltonian yields best results if both β and $\lambda \propto \beta/U^{1/2}$ are taken to the limit $\beta \to \infty$, as was done for the *t-J* model.

Generalizations for spins $1, \frac{3}{2}, \ldots$ or equivalently for soft-core bosons are effected by incorporating higher powers $(\sigma^\dagger d)^2, (\sigma^\dagger d)^3, \ldots$ onto the spin-$\frac{1}{2}$ mapping and adjusting the norms accordingly. Space does not permit further elaboration here, but these extensions are obvious.

In conclusion, we have illustrated a method, and several implementations of it, for exorcising the hard-core interaction in the many-body problem. Our procedure appears to be complementary to existing theories [11] in which auxiliary fields—"slave bosons" or "slave fermions"—keep track of local valency. Whenever such theories are implemented they invariably require decouplings or saddle-point approximations which enforce the hard-core constraints only *on average.* A ground-state energy calculated by such means is neither an upper nor a lower bound and cannot be used as a gauge of accuracy.

On the other hand, in the procedure outlined in the present paper, *any* simple phantom trial function satisfies the constraints exactly. Hence the Rayleigh-Ritz principle always applies. The parameters in our map must be chosen with some care, to optimize the low-lying states. We have given several examples above. Numerical and analytical approximate solutions of other models of particles on a lattice are under way and will be presented in due course.

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