Finite Hermitian alternatives to the Dyson Hamiltonian

E. R. Marshalek
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556
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It is pointed out that the nonunitary generalized Dyson mapping, which does not preserve Hermitian conjugation, is not necessary in order to obtain finite images of shell-model operators. Unitary mappings, which do preserve Hermitian conjugation, have long been available but largely overlooked.

Microscopic boson mappings,[1] while not the height of fashion, have greatly increased in popularity in recent years, propelled in part by the need for providing a foundation for the very successful phenomenological interacting boson model (IBM).[2] The generalized Dyson mapping of shell-model operators onto finite boson polynomials has been highly recommended[3] as superior to its close kin, the generalized Holstein-Primakoff (GHP)[4,5] and Marumori expansions,[6] which, in general, map onto infinite series in boson polynomials, thereby complicating the calculation of matrix elements. Unlike the infinite expansions, however, the Dyson mapping has the drawback that it does not preserve operator relations under Hermitian conjugation (HC); the Dyson Hamiltonian, for example, is not Hermitian. This drawback is not very serious, for, as shown by Takada, the non-Hermitian eigenvalue problem can be transformed in a relatively simple way into an equivalent Hermitian one.[7] With no intention of detracting from the virtues of the Dyson mapping, the purpose of this note is to point out alternative mappings that both preserve HC and are effectively finite, but have been by and large overlooked. In fact, these unitary mappings for systems with even particle numbers were already provided in the seminal paper of Janssen *et al.*,[5] who derived all of the mappings under discussion and their interrelations. The unitary mappings were extended to odd-particle systems by Marshalek[8] and Okubo,[9] who first pointed out the simplicity of the resulting Hamiltonian. The only applications were made by Hirsekorn and Weigert some years ago to light nuclei.[10] The more recent literature,[3,7] apparently oblivious to these earlier developments, gives the impression that the Dyson mapping is the only finite one. Actually, there is yet another type of finite unitary mapping, called a generalized Schwinger mapping,[11] but its applicability so far has been limited to particle-hole excitations of closed-shell systems, and it will not be further discussed here. Finally, it is worthwhile mentioning a simple trick proposed by Park,[12] which has been recently implemented in numerical calculations by Kuchta.[13] As discussed below, this trick gives a finite Hermitian Hamiltonian independently of which boson mapping is used, but may have drawbacks of its own. It should be emphasized that all of these methods are equivalent to each other and to the original many-fermion problem. Differences may arise, however, when truncated approximation schemes are invoked.

In the remainder of the paper, the relations between the different boson mappings will be briefly outlined, and some of the possibilities for finite-boson expansions discussed. For brevity, the discussion is limited to systems of even particle number, but the generalization to odd particle number is straightforward.[9]

It is well known that the set of all pairs of fermion creation and annihilation operators defined on a shell-model Fock space of n single-particle orbitals generates the Lie algebra corresponding to the group SO($2n$), while incrementing this set with the individual creation and annihilation operators themselves generates SO($2n+1$). The Fock space carries the solitary spinor irreducible representation (irrep) of SO($2n+1$) and the two spinor irreps of SO($2n$) corresponding to even- and odd-particle numbers. In the boson-mapping method, a boson (or, in the case of odd systems, a boson-fermion) realization of the algebra is defined on a subspace of an "ideal" space. This subspace, which is called the *physical subspace* and denoted here by $\mathcal{I}_P$, is the carrier of the spinor irreps in the ideal space, i.e., it is a replica of the fermion space. The non-null orthogonal complement of $\mathcal{I}_P$, which has nothing to do with fermions, is called the unphysical subspace; it is nothing more than "noise."

Now, one can define an invertible mapping operator V such that for any fermion state $|\rangle, V|\rangle = |)$, where $|)$ is the corresponding boson state in $\mathcal{I}_P$. The inverse V^{-1} can be defined so that it annihilates unphysical boson states, giving rise to the relations $V^{-1}V = 1_F$, where 1_F is the identity in the fermion space, and $VV^{-1} = P$, where P is the projector to $\mathcal{I}_P$. In the case of the Dyson mapping, $V^{-1} \neq V^{\dagger}$, so that the mapping is not isometric (i.e., the norms of vectors are not preserved). This is the origin of the violation of HC. For any fermion operator F, there is a corresponding operator in the ideal space given by $VFV^{-1} = PF_DP$, where F_D is the Dyson operator. Because of the violation of HC, the Dyson representation of the SO($2n$) algebra is not unitary. However, since the representation is finite dimensional, it can be unitarized by means of a similarity transformation: $F_U = SF_DS^{-1}$, where $PSP = SP = PS$ and likewise for S^{-1}. Thus, one can define an isometric mapping operator $U = SV$, called the Marumori operator, satisfying $U^{\dagger}U = 1_F$ and

$UU^\dagger = P$, such that for any fermion operator F,

$$F_M \equiv UFU^\dagger = PF_U P \ , \qquad (1)$$

where F_M is the Marumori image of F and both the images F_M and F_U preserve HC. The Marumori images should be distinguished from the infinite Marumori *expansion*, which is obtained by expressing the projector P in terms of bosons and writing (1) in normal order. It should also be noted that in Eq. (1) P may be dropped on the left if and only if $\mathcal{I}_\mathbf{P}$ is invariant under F_U, and on the right if and only if the unphysical subspace is so invariant. The projector P commutes with F_U if and only if both subspaces are invariant, i.e., the ideal space is reduced by F_U. It is also important that F_U in (1) may not be unique; several possibilities may exist that are equivalent in $\mathcal{I}_\mathbf{P}$ as discussed below.

Let $c_i^\dagger, c_i$, $i = 1, \ldots, n$ denote the fermion creation and annihilation operators and let $b_{ij}^\dagger, b_{ij}$ denote the boson creation and annihilation operators, labeled by fermion-pair quantum numbers and obeying the antisymmetry condition $b_{ji} = -b_{ij}$ (and H.c. equation) as well as the commutation relations

$$\begin{aligned} &[b_{ij}^\dagger, b_{kl}^\dagger] = 0 \quad \text{(and H.c. equation)} \ , \\ &[b_{ij}, b_{kl}^\dagger] = \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk} \ . \end{aligned} \qquad (2)$$

Then the Marumori representation of bifermion operators is given by[5,9]

$$(c_i^\dagger c_j)_M = \sum_k b_{ik}^\dagger b_{jk} P = P \sum_k b_{ik}^\dagger b_{jk} \ , \qquad (3)$$

$$\begin{aligned} (c_i^\dagger c_j^\dagger)_M &= P\mathcal{B}_{ij}^\dagger (1 + 2\hat{N}_B)^{-1/2} \\ &= \mathcal{B}_{ij}^\dagger (1 + 2\hat{N}_B)^{-1/2} P && (4a) \\ &= P b_{ij}^\dagger (1 + 2\hat{N}_B)^{1/2} && (4b) \\ &= P\{\mathbf{b}^\dagger [\mathbf{I} - (\mathbf{b}^\dagger \mathbf{b})^T]^{1/2}\}_{ji} \ , && (4c) \end{aligned}$$

$$(c_j c_i)_M = (c_i^\dagger c_j^\dagger)_M^\dagger \ , \qquad (5)$$

where

$$\mathcal{B}_{ij}^\dagger \equiv b_{ij}^\dagger - \sum_{kl} b_{ik}^\dagger b_{jl}^\dagger b_{kl} = (c_i^\dagger c_j^\dagger)_D \qquad (6)$$

and

$$\hat{N}_B \equiv \tfrac{1}{2} \sum_{ij} b_{ij}^\dagger b_{ij} \ . \qquad (7)$$

It should first be noted that the mapping of the density operators (3) is unique; it is the same for the Dyson and unitary mappings. On the other hand, there are three distinct forms for the unitary mapping of the pair-creation operators given by Eqs. (4), the last of which corresponds to the GHP, written in matrix form, where $(\mathbf{b}^\dagger)_{ij} = b_{ji}^\dagger$, T stands for the transpose, and $\mathbf{I}$ is the identity matrix. The GHP form is to be understood as an infinite expansion, which is useful for obtaining *perturbative* corrections to the random-phase approximation. It is the other two forms, (4a) and (4b), which are effectively finite in any basis of eigenfunctions of the boson number operator (7), that are of primary interest. The Dyson mapping of the pair-creation operators is given by Eq. (6), while that of the pair-annihilation operators is simply given by $(c_j c_i)_D = b_{ij} \neq (c_i^\dagger c_j^\dagger)_D^\dagger$.

The Marumori image of a number-conserving Hamiltonian containing two-body particle-hole (p-h) and particle-particle (p-p) interactions, such as the quadrupole-quadrupole plus pairing interactions, is given by

$$\begin{aligned} H_M = &\sum_{ij} \epsilon_{ij} (c_i^\dagger c_j)_M + \tfrac{1}{2} \sum_{ijkl} F_{ij,kl} (c_i^\dagger c_k)_M (c_j^\dagger c_l)_M \\ &+ \tfrac{1}{4} \sum_{ijkl} G_{ij,kl} (c_i^\dagger c_j^\dagger)_M (c_l c_k)_M \ , \end{aligned} \qquad (8)$$

where the first term on the right is the single-particle Hamiltonian, $F_{ij,kl}$ is the unantisymmetrized p-h matrix element, and $G_{ij,kl}$ is the antisymmetrized p-p matrix element. For the single-particle Hamiltonian and the p-h interaction, Eq. (3) gives a finite Hermitian form that reduces the ideal space and consists of one- and two-body boson interactions, for both the Dyson and unitary mappings. For the p-p interaction, the situation is more complicated. First of all, the Dyson mapping gives

$$(V_{pp})_D = \tfrac{1}{4} \sum_{ijkl} G_{ij,kl} \mathcal{B}_{ij}^\dagger b_{kl} P \ , \qquad (9)$$

which is not Hermitian. Incidentally, this result can be obtained by combining the unitary mapping (4a) with the H.C. of the second form (4b), which, of course, violates HC. On the other hand, if one consistently uses either (4a) or (4b) and the corresponding H.c. equation, one finds the following two finite Hermitian mappings:

$$\begin{aligned} (V_{pp})_M &= \tfrac{1}{4} \sum_{ijkl} G_{ij,kl} \mathcal{B}_{ij}^\dagger (1 + 2\hat{N}_B)^{-1} \mathcal{B}_{kl} \overleftrightarrow{P} \ , && (10a) \\ &= P \tfrac{1}{4} \sum_{ijkl} G_{ij,kl} b_{ij}^\dagger (1 + 2\hat{N}_B) b_{kl} P \ , && (10b) \end{aligned}$$

where $\overleftrightarrow{P}$ indicates that the projector P can be commuted to the left side of the sum. It should be noted that the number of bosons is a constant of the motion. Then the mapping (10a), which has not been discussed before, effectively gives rise to three-body boson interactions, as well as one- and two-body interactions. The Hamiltonian has the nice property of not coupling the physical and unphysical subspaces even without the projector. The result (10b), which was first noted by Okubo,[9] is particularly simple in that it effectively involves only one-body boson terms. However, this simplicity carries a price: The projectors on both sides of the right-hand side of (10b) must be maintained. Without them, the Hamiltonian would couple physical and unphysical vectors and give rise to completely spurious results. This circumstance would cause no difficulties in applications in which the Hamiltonian is diagonalized in a truncated basis of physical states constructed beforehand, as has been the case in most of the applications of the Dyson mapping. Moreover, (10b) is simpler than the Dyson mapping (9). In other applications, such as mean-field approximations, (10b) would probably be disadvantageous, while (10a) might be quite useful.

Another way to achieve a finite Hermitian form for the Hamiltonian (8) is provided by the Park-Kuchta trick.[12,13] Here, the p-p interaction is rearranged into a p-h interaction by writing

$$c_i^\dagger c_j^\dagger c_l c_k = \delta_{lj} c_i^\dagger c_k - c_i^\dagger c_l c_j^\dagger c_k \ . \tag{11}$$

Then, the Hamiltonian can be written entirely in terms of the density operators (3), which are the generators of the subgroup $U(n)$. The resulting boson Hamiltonian, which is compatible with all mappings, then contains only one- and two-body terms and is given by

$$H_M = \left[\sum_{ijk} \left[\epsilon_{ij} + \tfrac{1}{2} \sum_l F_{il,lj} \right] b_{ik}^\dagger b_{jk} + \tfrac{1}{2} \sum_{ijkl} \mathcal{V}_{ij,kl} b_{ij}^\dagger b_{kl} + \tfrac{1}{2} \sum_{ijklmn} \mathcal{V}_{ij,kl} b_{im}^\dagger b_{jn}^\dagger b_{km} b_{ln} \right] \vec{P} \ , \tag{12}$$

where

$$\mathcal{V}_{ij,kl} \equiv F_{ij,kl} + \tfrac{1}{2} G_{ij,kl} \ . \tag{13}$$

As indicated, the Hamiltonian in brackets cannot couple physical and unphysical states. The recoupling of the p-p interaction into a p-h interaction has the drawback of obscuring the coherence properties that motivated the original decomposition of the interaction into p-p and p-h parts. Consequently, unless bosons of all angular momenta are utilized in the subsequent approximations, serious errors could result. However, this possibility seems to have been taken into account in Kuchta's treatment. Note that (10a) provides an alternative that does not scramble the coherence of the interaction.

The Park-Kuchta trick is obviously limited to number-conserving Hamiltonians. In the case of quasiparticle Hamiltonians, the number is not generally conserved. In that case, however, the unitary mappings (4a) or (4b) are still available and convenient to apply to any basis of boson number eigenstates. For example, the mapping of $(c_i^\dagger c_j^\dagger)_M (c_k^\dagger c_l^\dagger)_M$ and $(c_i^\dagger c_j^\dagger)_M (c_k^\dagger c_l)_M$ using Eqs. (4a), (4b), and (3) is no more difficult than in the number-conserving case, giving rise to at most three-body boson interactions, which is also the case for the quasiparticle Dyson mapping. In fact, an example of a quasiparticle application of (4b) is provided by the work of Hirsekorn and Weigert.[10]

With all of these mappings, it is important to distinguish physical and unphysical eigenvectors. One way to do this is to diagonalize only within (truncated) bases of boson vectors obtained by mapping fermion vectors, as in the work of Takada. If the basis used spans all or part of the unphysical subspace, it is essential to have an operator whose eigenvalues can distinguish physical and unphysical vectors. In principle, P could be used, but it is cumbersome to work with. Another possibility is provided by the operator S first introduced in Ref. 5 and advocated by Park.[12] This operator was implemented by Kuchta[13] as a constraint in the boson mean-field treatment to keep the wave function largely confined to $\mathcal{J}_P$. But there are many other alternatives to the S operator, such as the Casimir operator of SO($2n$), that could be used instead.

In conclusion, the mappings (4a) or (4b) provide effectively finite Hermitian Hamiltonians and in general preserve HC. For number-conserving Hamiltonians, the Park-Kuchta trick can also be useful if caution is exercised in subsequent approximations to maintain the coherence properties of the p-p interaction. Thus, the Dyson mapping is not the only one worth investigating.

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