Inadequacy of four-particle tests of Dyson boson mapping

G.-K. Kim and C. M. Vincent
Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
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The spurious state problem in generalized Dyson boson mapping is examined. For cases where the fermion space is restricted to at most four-quasiparticle excitations, we show that Dyson boson images of normal-ordered quasiparticle interactions have identically vanishing matrix elements in the unphysical boson space. This "decoupling" feature explains the finding of previous authors that, in systems with at most four quasiparticles, every spurious state appears at its unperturbed energy. However, we show that the decoupling property does not generally hold in problems where there are excitations of more than four quasiparticles. Claims about methods for the spurious state problem, even though verified in four-quasiparticle calculations, may therefore be of limited validity.

Dyson-type methods[1-3] of mapping the fermion problem into a boson space have begun to be used in studies of low-lying collective states in nuclei with even numbers of valence particles. The convenience of such methods is really a result of working in an enlarged space which includes states that violate the Pauli principle. In the ideal case where the calculations are done exactly, each of the resulting stationary states will be either "physical," so that it corresponds to an exact fermion eigenstate, or "spurious," so that it has no fermion counterpart at all. Approximations of good accuracy blur this distinction only slightly. Meaningful comparison with experiment requires one to identify and discard the spurious states. Ring and Schuck[2] show that their mode coupling theory (MCT) is equivalent to the generalized Dyson boson mapping.[1] They suggest that every spurious state reveals itself by its energy, which is a sum of free-quasiparticle energies, and they verify that this "decoupling" property indeed holds in actual four-particle, four-hole, and two-particle-two-hole[4] test cases. Similarly, in a study of four particles with a quadrupole-quadrupole Hamiltonian in a single j shell, Geyer and Lee[3] found that for the non-Hermitian choice of Dyson boson Hamiltonian (obtained by Dyson mapping the normal-ordered fermion Hamiltonian), the spurious states are easily identified because the corresponding eigenenergies are all zero.

Tests based on such cases seem intuitively quite convincing, because they do contain spurious states. However, to be reliable such tests must allow the two-body interaction the same ability to couple the spurious states to the physical space that it has in larger problems. The cases mentioned above turn out to be deficient in this regard.

These cases can be compactly treated together, as special cases of a system of up to four (Hartree-Fock) quasiparticles. We will show, in fact, that the "decoupling" property of the spurious states noted by Ring and Schuck and by Geyer and Lee holds for systems of at most four quasiparticles *and is limited to them.*

Let $\alpha_i^\dagger$ and α_i be anticommuting quasiparticle creation and annihilation operators, which satisfy

$$\{\alpha_i,\alpha_j^\dagger\}=\delta_{ij},\quad \alpha_i|0\rangle_F=0\ , \tag{1}$$

where $|0\rangle_F$ is the quasiparticle vacuum. In the Dyson boson mapping method, ideal boson creation and annihilation operators $b_{ij}^\dagger$ and b_{ij} are introduced; these are antisymmetric in their indices, so that

$$\begin{aligned} &b_{ij}^\dagger=-b_{ji}^\dagger\ ,\\ &[b_{ij},b_{kl}^\dagger]=\delta_{ik}\delta_{jl}\quad (i<j,k<l)\ ,\\ &b_{ij}|0\rangle=0\ , \end{aligned} \tag{2}$$

where $|0\rangle$ is the boson vacuum. The *physical* boson space L_P is generated by repeated applications of Pauli-corrected boson operators

$$B_{ij}^\dagger=b_{ij}^\dagger-\sum_{kl}b_{ik}^\dagger b_{jl}^\dagger b_{kl}\ . \tag{3}$$

Every state in L_P is fully antisymmetric in its boson indices. Let P be the orthogonal projection operator on L_P, and define $Q=1-P$ so that $PQ=0$. The operator Q projects on the unphysical (i.e., spurious) space L_Q. The Dyson image $(\Theta)_D$ of a fermion operator Θ is given by[1]

$$(\Theta)_D=\overline{\Theta}P\ , \tag{4}$$

where $\overline{\Theta}$ is a boson operator obtained by the replacement

$$\begin{aligned} &\alpha_i^\dagger\alpha_j^\dagger\rightarrow B_{ij}^\dagger\ ,\\ &\alpha_j\alpha_i\rightarrow b_{ij}\ ,\\ &\alpha_i^\dagger\alpha_j\rightarrow\sum_k b_{ik}^\dagger b_{jk}\ . \end{aligned} \tag{5}$$

If one actually uses the mapping (4), the presence of the projection operator P ensures that all spurious eigenstates will be at zero energy. However, the practical convenience of the Dyson boson representation depends on working in the full boson space and replacing (4) by the simpler transformation

$$\Theta\rightarrow\overline{\Theta}\ , \tag{6}$$

defined by (5). Equation (5) also preserves the bifermion commutation relations.

We now establish the decoupling property. For two quasiparticles no spurious states occur, because

$$b_{ij}^\dagger|0\rangle=B_{ij}^\dagger|0\rangle\in L_P \text{ for all } i \text{ and } j\ . \tag{7}$$

The four-quasiparticle problem is the simplest case in which L_Q is not a null space. Let us consider the quasiparticle representation of a general fermion Hamiltonian with two-body interaction[5]

$$H = H_0 + V \ , \tag{8}$$

where

$$H_0 = \sum E_i \alpha_i^\dagger \alpha_i \ , \tag{9}$$

$$V = \sum_{ijkl} [(v_{ijkl}^{40} \alpha_i^\dagger \alpha_j^\dagger \alpha_k^\dagger \alpha_l^\dagger + \text{H.c.}) + (v_{ijkl}^{31} \alpha_i^\dagger \alpha_j^\dagger \alpha_k^\dagger \alpha_l + \text{H.c.}) + \tfrac{1}{4}(v_{ijkl}^{22} \alpha_i^\dagger \alpha_j^\dagger \alpha_k \alpha_l)] \ . \tag{10}$$

Note that all the operators in H are normal ordered in the quasiparticle operators. Now let us consider calculations restricted to a space of up to four-quasiparticle excitations. This means that the boson space is limited to states of at most two bosons. Within this restricted space, we shall show that

$$Q\overline{V} = 0 \ . \tag{11}$$

We prove (11) for operators of the types v^{40} and v^{22}; similar arguments apply to the remaining types of operators in (10). By Eq. (5) we have

$$V^{40} = \overline{\alpha_i^\dagger \alpha_j^\dagger \alpha_k^\dagger \alpha_l^\dagger} = B_{ij}^\dagger B_{kl}^\dagger \ . \tag{12}$$

The only nonvanishing matrix elements of V^{40} in the four-quasiparticle space are of the type $\langle 2 \text{ boson} | V^{40} | 0 \rangle$. Since $|0\rangle$ is a physical state and $B_{ij}^\dagger$ gives a physical state when acting on any physical state, we have

$$QV^{40} = 0 \ . \tag{13}$$

For the v^{22} term,

$$V^{22} = \overline{\alpha_i^\dagger \alpha_j^\dagger \alpha_k \alpha_l} = B_{ij}^\dagger b_{lk} \ . \tag{14}$$

For any state ϕ within the restricted space of 0-, 1-, and 2-boson states,

$$b_{ij}\phi \in L_P \ , \tag{15}$$

since $b_{ij}\phi$ is a linear combination of $|0\rangle$ and a one-boson state, both of which are physical states. Since $B_{ij}^\dagger$ transforms every physical state into a physical state, Eqs. (14) and (15) imply that

$$QV^{22} = 0 \ . \tag{16}$$

Equations (13) and (16), together with similar relations for the v^{31} terms, establish the decoupling property (11). This equation implies that the spurious states will be decoupled, i.e., $Q\overline{V}P = 0$, and have noninteracting energies, because $Q\overline{V}Q = 0$. The value of $P\overline{V}Q$ is immaterial. Each spurious eigenvalue of H is an eigenvalue of H_0, given by a sum of free quasiparticle energies E_i. This conclusion, one must remember, depends on the fact that H is written in normal-ordered form. Thus we have explained the findings of Ring and Schuck and Geyer and Lee.

To see that the decoupling property, Eq. (11), does *not* hold generally for more than four fermions, it is sufficient to consider one very specific example, say the following three-boson state (corresponding to six fermions),

$$\phi_3 = (b_{ij}^\dagger)^2 b_{kl}^\dagger |0\rangle \ . \tag{17}$$

(This state is *entirely* spurious because antisymmetrization of its indices annihilates it.) Now consider the action on ϕ_3 of $B_{mn}^\dagger b_{ij}$, a typical term of $\overline{V}$, and for simplicity suppose that i, j, k, l, m, and n are all distinct. We have

$$\psi = B_{mn}^\dagger b_{ij}\phi_3 = 2B_{mn}^\dagger b_{ij}^\dagger b_{kl}^\dagger |0\rangle = 2\left(b_{mn}^\dagger - \sum_{pq} b_{mp}^\dagger b_{nq}^\dagger b_{pq} \right) b_{ij}^\dagger b_{kl}^\dagger |0\rangle \ . \tag{18}$$

When this is expressed solely in terms of creation operators $b^\dagger$, it becomes evident that ψ is not fully antisymmetric; for example, the interchange of m with i does not simply reverse the sign of ψ. Consequently, ψ has a nonvanishing spurious component,

$$Q\psi = QB_{mn}^\dagger b_{ij}\phi_3 \neq 0 \ , \tag{19}$$

in contradiction with Eq. (11). Other counterexamples are easy to construct.

In conclusion, we see that past findings[3,4] on the spurious state problem are explained by the "decoupling" result (11), which implies that the Dyson image of a normal-ordered two-body interaction vanishes in the unphysical space. The limitation of this result to systems of at most four quasiparticles prevents useful generalization of those findings. Moreover, caution seems advisable also in cases where four-particle tests are used for other methods, such as the boson-fermion hybrid theory of Wu and Feng.[6]

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