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Method for treating the spurious center of mass problem in a dynamically determined basis

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When a basis space for diagonalizing a multiparticle Hamiltonian is dynamically determined from a set of variational calculations, it is then possible to treat the spurious center of mass motion problem at a level consistent with the treatment of the full solution of the problem. We propose a practical systematic method based on double diagonalization within a variationally determined subspace. The proposed method converges to an exact treatment when the variationally determined subspace spans the full model space.

[NUCLEAR STRUCTURE Spurious center of mass problem; correction to shell model bases; correction to variationally determined bases.]

When one attempts to obtain the eigenstates of a many body Hamiltonian in a large configuration space, either exactly or approximately, one is often confronted with the possibility of having spurious states in the spectrum.[1-5] Spurious states will be present if the center of mass of the many particle system is not confined to a particular state of motion. Since most calculations of the eigenstates of the Hamiltonian operator are performed with basis states which are not simultaneously eigenfunctions of a center of mass operator (e.g., in a basis constructed from single particle states), spurious states may occur even in the case when only the intrinsic Hamiltonian operator

$$\hat{H}_{\text{int}} = \hat{H} - \hat{H}_{\text{c.m.}}$$

has been used.

One method to remove the spurious states is to restore translational invariance through the requirement that the eigenstates of the Hamiltonian operator be eigenstates of the operator $\hat{P}_{\text{c.m.}}$ with the same eigenvalue.[1] This procedure, which is formally and physically correct, may, however, be extremely difficult to apply in realistic calculations.

A somewhat different approach for the removal of the spurious states, which may be more applicable in calculations of the eigenstates of a Hamiltonian defined in a finite dimensional model space, is first to diagonalize $H_{\text{c.m.}}$ in this model space and then to use a set of degenerate (or nearly degenerate) eigenstates of $H_{\text{c.m.}}$ to diagonalize $\hat{H}$ or $\hat{H}_{\text{int}}$. This double diagonalization procedure for eliminating states of c.m. excitation is equivalent to projecting the eigenstates onto a subspace of states with the same c.m. motion. Although translational invariance has not been restored, spurious states will be removed from the eigenvalue spectrum and the subsequent errors in the calculation of the intrinsic eigenvalue spectrum for the lower-lying eigenstates should be negligible in most cases.

Sometimes, the full double diagonalization required may be difficult if not impossible to carry out due to the size of the model space. For very large configuration spaces, we would like to point out that a tractable means for removing spurious states may be incorporated into a recently proposed general method for obtaining a systematically improved description of the lower-lying eigenstates via configuration mixing calculations with basis states generated from variational methods.[6-8] The basic idea in this approach is to construct sequentially a set of basis states all of which are solutions of a set of variational equations and whose variational energies form a monotonically increasing sequence. States generated in this dynamical manner are ideally suited for configuration mixing calculations yielding rapid convergence to the lower end of the eigenvalue spectrum. Since these basis states need not be confined to a particular state of c.m. motion, spurious states can occur. We may sequentially remove these spurious states in a manner analogous to that indicated above by a prediagonalization of $\hat{H}_{\text{c.m.}}$ in the subspace spanned by the set of variationally determined basis states. At each step of the basis generation, spurious states are identified by a lack of degeneracy in the eigenstates of $\hat{H}_{\text{c.m.}}$. Furthermore, it is interesting to note that in the case where the variationally

determined space spans the full model space, the present approach is equivalent to the full double diagonalization approach.

It is reasonable to argue that the lower-lying variationally determined states are not likely to differ by a spurious c.m. excitation. For example, in variational calculations of the ground state in the Hartree-Fock approach it is generally conceded that unphysical contributions for spurious c.m. excitations do not appear to be a serious problem particularly in systems with a large number of particles.[9,10] If such is the case, the above procedure will simply serve as a method to check for spurious states.

We believe this method of obtaining the low-lying eigenstates free of spurious c.m. excitations will be particularly useful for calculations performed in large model spaces. In such cases, the task of diagonalizing $\hat{H}_{\text{c.m.}}$ should incur little additional effort yet resolve the spurious center of mass motion problem.

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