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A Reformulation of the Mode-Coupling Method.

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In the last few years several attempts have been made to include the two-particle and particle-hole correlated states as basis states in the description of nuclear spectra ^(1,2). In particular, it has been shown that the weak-coupling model (WCM) reproduces well the exact shell-model calculated states in ²⁰⁸Pb ⁽²⁾. It has also been proved that the mode-coupling method (MCM) gives the exact shell-model energies in a number of situations ⁽¹⁾. The MCM formalism is, however, much simpler than the one in the WCM. The main reason for this simplicity is that the two-body bare interaction does not appear in the MCM. Nevertheless, there are a few drawbacks with the MCM which are not present in other models, namely,

i) the overcomplete set of basis states provides a number of spurious states which may not be easily disentangled from the physical states in realistic calculation, where the basis has generally to be truncated (drawback shared by the nuclear field theory ⁽³⁾);

ii) the matrix that provides the energies is not Hermitian and complex solutions may be obtained;

iii) it is not clear how to calculate the wave functions, for which arbitrary normalization conditions have so far been used ⁽¹⁾.

In this letter we reformulate the MCM to avoid the three drawbacks mentioned above while keeping the essential positive features of the model. To make the presentation clear we analyse the simple case of nuclei with three particles outside a closed-shell core.

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The basis set of states are denoted by $|b\rangle \equiv (c_i^\dagger P^+(\alpha))_J |0\rangle$, where $c^\dagger$ is the usual fermion creation operator and the two-particle TDA wave function is given by

$$(1) \quad |\alpha\rangle = P^+(\alpha)|0\rangle = \sum_{ij} X(ij; \alpha) (c_i^\dagger c_j^\dagger) \lambda_\alpha \mu_\alpha |0\rangle.$$

Inserting the two- into the three-particle TDA equation, one gets the MCM eigenvalue equation ⁽¹⁾

$$(2) \quad \sum_{b'} M(b, b') \langle nJ|b'\rangle = W(nJ) \langle nJ|b\rangle,$$

where $|nJ\rangle$ is the three-particle wave function with energy $W(nJ)$ and

$$(3) \quad M(b, b') = (\varepsilon_i + \omega_\alpha) \delta_{ii'} \delta_{\alpha\alpha'} + \sum_k (\omega_{\alpha'} - \varepsilon_k - \varepsilon_i) A_k(b, b').$$

The quantity

$$(4) \quad A_k(b, b') = \lambda_\alpha \lambda_{\alpha'} \begin{Bmatrix} j_i & j_k & \lambda_{\alpha'} \\ j_{i'} & J & \lambda_\alpha \end{Bmatrix} (1 + \delta_{ki'})^\dagger X^*(ki'; \alpha) (1 + \delta_{ki})^\dagger X(ki; \alpha')$$

is related to the overlap between the basis states as

$$(5) \quad \langle b|b'\rangle = \delta_{ii'} \delta_{\alpha\alpha'} + \sum_k A_k(b, b').$$

In these equations ε is the single-particle energy and ω is the two-particle TDA energy. The rest of the notation is standard.

The basis set of states $\{b\}$ is overcomplete because it does not fully contain the Pauli principle. Hence the diagonalization of eq. (2) does not provide the three-particle wave function $|nJ\rangle$ unless the Pauli principle condition is somehow added to (2). The energies $W(nJ)$ are nevertheless correctly given by the MCM because they are not affected by the transformation from the uncoupled TDA equation (which fully includes the Pauli principle) to eq. (2). However, a number of spurious solution—with unperturbed energy values $\varepsilon + \omega$ —are also given by the MCM according to the degree of overcompleteness. Moreover, the matrix M is not Hermitian.

To overcome these problems we first diagonalize the Hermitian overlap matrix (5) (which is calculated at the same time than the matrix M , according to eq. (3)). The eigenstates with eigenvalue $\lambda_m \neq 0$ provide a complete and orthonormal set of states $|m\rangle = \sum_b \xi_m(b) |b\rangle$ (see ref. ⁽²⁾). One can then write eq. (2) as

$$(6) \quad \sum_{m'} T(m, m') \langle nJ|m'\rangle = W(nJ) \langle nJ|m\rangle,$$

where the matrix

$$(7) \quad T(m, m') = \lambda_{m'} \sum_{bb'} \xi_m(b) M(b, b') \xi_{m'}^*(b')$$

is Hermitian since all W are real and the set of vectors $\{m\}$ is complete. In addition the matrix T has the proper number of dimensions and there is not any spurious solution.

The diagonalization of T provides the physical wave functions

$$(8) \quad |nJ\rangle = \sum_m \langle m|nJ\rangle |m\rangle$$

TABLE I. — *The states $\frac{9}{2}^+$ in ^{91}Nb calculated with the mode-coupling method as presented in this letter. In parenthesis the nuclear field theory wave functions. S_k is the one-particle transfer spectroscopic factor for the reaction $^{90}\text{Zr}(\text{gs}) \rightarrow ^{91}\text{Nb}(\frac{9}{2}^+)$. The overlap matrix (5) has in this case five degenerate eigenvalues $\lambda_m = 0$ while the other three are also degenerate with value $\lambda_m = 3$.*

E (MeV)	$g_{\frac{1}{2}} \otimes 0_1^+$	$g_{\frac{3}{2}} \otimes 0_2^+$	$g_{\frac{5}{2}} \otimes 2^+$	$g_{\frac{7}{2}} \otimes 4^+$	$g_{\frac{9}{2}} \otimes 6^+$	$g_{\frac{11}{2}} \otimes 8^+$	$p_{\frac{1}{2}} \otimes 4^-$	$p_{\frac{3}{2}} \otimes 5^-$	S_k
—20.654	0.29 (—5.23)	—0.26 (—2.71)	0.32 (—0.09)	0.04 (0.03)	—0.09 (0.10)	—0.12 (0.15)	—0.14 (—3.91)	—0.16 (1.18)	0.96
—18.953	—0.19 (—2.11)	0.17 (3.36)	0.00 (—1.19)	—0.31 (0.40)	—0.14 (1.39)	—0.20 (2.08)	—0.22 (—0.23)	—0.26 (0.07)	—0.26
—17.870	—0.00 (—0.02)	0.00 (0.02)	0.00 (—0.23)	—0.00 (—0.19)	—0.11 (0.63)	0.37 (—0.25)	—0.41 (0.00)	0.13 (0.00)	—0.01

which defines the normalization condition

$$(9) \quad \delta_{nn'} \delta_{JJ'} = \sum_m \langle m | nJ \rangle \langle m | n'J' \rangle^*.$$

Finally, the amplitude $\langle nJ | b \rangle$ of eq. (2)—which is also the one-particle transfer spectroscopic amplitude for the process $|\alpha\rangle \rightarrow |nJ\rangle$ —is given by

$$(10) \quad \langle nJ | b \rangle = \sum_m \langle nJ | m \rangle \langle m | b \rangle = \sum_m \lambda_m \xi_m^*(b) \langle nJ | m \rangle.$$

We applied this method to the analysis of the spectrum of ^{91}Nb , *i.e.* three protons outside the ^{88}Sr core. The single-particle states are $1p_{\frac{1}{2}}$ and $0g_{\frac{7}{2}}$. The single-particle energies and the states in ^{90}Zr were taken from ref. (4), where it is shown that the shell-model gives a good account of the experimental data.

We did the same calculation in the framework of the nuclear field theory, for which a method is also available to obtain the exact shell-model physical quantities (5).

We found in all cases that the results of both the NFT and the MCM as presented in this letter, coincide with the shell-model calculation for the energies as well as for the spectroscopic factor amplitudes (10).

As an example, we show in table I the $\frac{9}{2}^+$ states. The NFT and the MCM wave functions differ very much from each other. This is understandable since in an over-complete space the components of a vector are not uniquely determined.

While both methods give the exact result one must say, however, that the MCM calculation is much easier to perform than the full NFT calculation.

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