Numerically exact description of multicluster bound states(*)

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Summary. — We present the variational few-body approach to multiparticle bound states called the correlated-Gaussian stochastic variational method (CGSVM) and show how it can be applied to systems of nuclear clusters. It will be demonstrated that the treatment of the intercluster motion is numerically exact and the method provides a virtually perfect realization of the conventional cluster model.

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1. – Introduction

Some light nuclei do not seem to obey mean-field theories; they rather behave as composites of smaller clusters. For example, the light multi-$\alpha$ nuclei and halo nuclei show clustering even in their ground states. The clusters are subsystems whose internal bindings are much stronger than the binding between them, and thus the behaviour of a multi-cluster system is mostly determined by the intercluster relative motion. Therefore, while the cluster internal states may be described schematically, the relative motion should be treated as accurately as possible.

It is a challenge to describe multicluster systems accurately. To cope with the technical difficulties, one may divide the system into as few clusters as possible, running the risk of including very soft clusters, or one may admit just well-behaved clusters at the cost of having many. E.g., the $^9$Li+n+n model of $^{11}$Li involves a distortable $^9$Li, while an $\alpha+t+n+n+n+n$ model involves six clusters. We opt for the latter strategy, and present a framework in which the intercluster motion is treated virtually exactly.

In sect. 2 we outline the theoretical framework, in sect. 3 we show how the method works when all clusters are structureless, in sect. 4 we test the cluster ansatz for the example of $^6$He, and in sect. 5 we draw some general conclusions.

2. – Theory

The approach to be presented [1] is based on a variational method with a trial function built up from generalized Gaussians called correlated Gaussians. We introduce this trial function with elementary considerations and start with a structureless particle.

Choosing a suitable trial function amounts to choosing a functional form that is likely to approximate a wave function of any conceivable shape with as few parameters as possible. A radial wave function \( F_{lm}(r) \) is most conveniently expressed as \( F_{lm}(r) \approx \sum_k c_k g_{\alpha_k}(r) \), where \( g_{\alpha_k}(r) \) is a function containing a continuous parameter \( \alpha \). A nodeless harmonic-oscillator (h.o.) function \( g_{\alpha}(r) = r^l \exp[-\frac{1}{2}a r^2] \) is qualified for this role because any (square-integrable) wave function with angular momentum \( lm \) can be approximated, to any desired accuracy, by a linear combination of such functions: \( F_{lm}(r) \approx \sum_{k=1}^M c_k \cdot \exp[-\frac{1}{2}a r^2] Y_{lm}(r) \), with \( Y_{lm}(r) = r^l Y_{lm}(r) \). For an \( A \)-particle problem, one should introduce a set of intrinsic Jacobi coordinates \( x_1, \ldots, x_{A-1} \), to be regarded as a column vector \( x \). We exclude the vector pointing to the total centre of mass (c.m.) from the outset to emphasize that the dynamics of the problem can be solved without reference to the c.m.

The expansion may then take the form

\[
F_{LMx}(x) \approx \sum_{\{k\}} c_{\{k\}} \exp \left[ -\frac{1}{2} \sum_{i=1}^{A-1} a_{\{k\}ij} x_i^2 \right] \theta_{\{l\}LMx}(x) = \sum_{\{k\}} c_{\{k\}} \exp \left[ -\frac{1}{2} \tilde{x} A_{\{k\}} x \right] \theta_{\{l\}LMx}(x).
\]

Here \( \{k\} \equiv \{k_1, \ldots, k_{A-1}\} \) label the different sets of product Gaussians, which are, in the second line, written as a quadratic form with \( A_{\{k\}} \) a diagonal matrix: \( A_{\{k\}ij} = a_{\{k\}ij} \delta_{ij} \). The tilde marks transposition, and the quadratic form \( \tilde{x} A_{\{k\}} x \) involves scalar products of the Cartesian vectors: \( \tilde{x} A_{\{k\}} x = \sum_i x_i \cdot (\sum_j A_{\{k\}ij} x_j) \). The factor \( \theta_{\{l\}LMx}(x) \) may be imagined as a vector-coupled product of the solid spherical harmonics for the individual Jacobi vectors; then the label \( \{l\} \) may denote a set of orbital momentum quantum numbers:

\[
\theta_{\{l\}LMx}(x) = [Y_{l_1}(x_1) \ldots Y_{l_{A-1}}(x_{A-1})]_{LMx}.
\]

The sum may contain far fewer terms than if there were \( A - 1 \) uncorrelated particles, owing just to the correlations that blur the mean-field picture.

To conform to some correlations or to some part of the asymptotic region, one may alternatively choose other sets of relative coordinates. E.g., for four identical particles there are two topologically different sets of independent relative vectors: those which form a K pattern (the Jacobi vectors) and those which form an H, with one particle sitting at the end of each arm. E.g., an asymptotic partitioning into two pairs of particles is described most economically with the H-shaped set of vectors. To have good asymptotics everywhere, it is economical to include terms with all possible relative vectors. Such terms will overlap with each other substantially, but since even the terms with the same relative vectors are non-orthogonal, this does not pose extra difficulties.

This scheme becomes simpler by two straightforward generalizations.

First, all possible relative coordinate systems, and even their mixtures, may be contained in a single sum as in eq. (2) if we allow \( A_{\{k\}} \) to be arbitrary positive-definite sym-