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A Nuclear Model with Explicit Mesons

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Abstract A nuclear model is proposed where the nucleons interact by emitting and absorbing mesons, and where the mesons are treated explicitly. A nucleus in this model finds itself in a quantum superposition of states with different number of mesons. Transitions between these states hold the nucleus together. The model—in its simplest incarnation—is applied to the deuteron, where the latter becomes a superposition of a neutron-proton state and a neutron-proton-meson state. Coupling between these states leads to an effective attraction between the nucleons and results in a bound state with negative energy, the deuteron. The model is able to reproduce the accepted values for the binding energy and the charge radius of the deuteron. The model, should it work in practice, has several potential advantages over the existing non-relativistic few-body nuclear models: the reduced number of model parameters, natural inclusion of few-body forces, and natural inclusion of mesonic physics.

1 Introduction

In the low-energy regime the nucleons are believed to interact by exchanging mesons [1–3]. However the accepted contemporary non-relativistic few-body nuclear models customarily eliminate mesons from the picture and introduce instead phenomenological meson-exchange-inspired nucleon-nucleon potentials tuned to reproduce available experimental data [3–6].

In this contribution the meson-exchange paradigm is going to be applied literally by allowing nucleons to explicitly emit and absorb mesons which will be treated on the same footing as the nucleons. A nucleus in this model will be a superposition of states with different number of emitted mesons.

Since it takes energy to generate a meson, in the low-energy regime the states with mesons will find themselves under a potential barrier equal to the total mass of the mesons. One might expect that in the first approximation only the state with one meson will contribute significantly.

In one-meson approximation a nucleus becomes a superposition of two subsystems: a subsystem with zero mesons, and a subsystem with one meson. The corresponding Hamiltonian is then given as a matrix,

$$H = \begin{pmatrix} K_N & W \\ W^\dagger & K_N + K_\sigma + m_\sigma \end{pmatrix}, \tag{1}$$

where K_N is the kinetic energy of nucleons, K_σ is the kinetic energy of the meson, m_σ is the mass of the meson, and W is the operator that couples these two subsystems by generating/annihilating the meson. The corresponding Schrodinger equation for the nucleus is then given as

$$\begin{pmatrix} K_N & W \\ W^\dagger & K_N + K_\sigma + m_\sigma \end{pmatrix} \begin{pmatrix} \psi_N \\ \psi_{\sigma N} \end{pmatrix} = E \begin{pmatrix} \psi_N \\ \psi_{\sigma N} \end{pmatrix}, \tag{2}$$

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where ψ_N is the wave-function of the subsystem with nucleons only; $\psi_{\sigma N}$ is the wave-function of the subsystem with nucleons and a meson; and E is the energy. If $E < m_\sigma$ the meson is under barrier and cannot leave the nucleus.

In the literature one can find several relativistic approaches to treat mesonic degrees of freedom dynamically [7,8]. As an alternative, this model attempts to use the (usually somewhat simpler) non-relativistic Schrödinger equation in line with the traditional phenomenological few-nucleon models.

The potential advantages of this model, should it work in practice, are the reduced number of parameters (possibly only few parameters per meson); natural inclusion of few-body forces (expected to arise from few-meson states); and natural inclusion of mesonic physics. One disadvantage is a substantially increased computational load: an N body problem becomes (at least) a coupled N plus $N+1$ body problem.

The lightest mesons are pions and they should presumably be included first. However in this first conceptual trial of the model we shall for simplicity only include the scalar-isoscalar sigma-meson [9] which is assumed to be responsible for the bulk of the intermediate-range attraction in nuclei [6] and which is also the lightest meson in relativistic mean-field theories [10].

In the next sections we shall (i) describe the practical application of the model to the deuteron; (ii) describe the correlated Gaussian method for coupled few-body systems to be used to solve the problem numerically; (iii) present the results for the deuteron; and (iv) give a conclusion. Several relevant formulae are collected in the "Appendix".

2 Deuteron as a System of Two Nucleons and a Meson

The deuteron in this model consists of two coupled subsystems: a two-body neutron-proton subsystem and a three-body neutron-proton-meson subsystem. The wave-function ψ of the deuteron is then a two-component structure,

$$\psi = \begin{pmatrix} \psi_{\rm np}(\mathbf{r}_{\rm n}, \mathbf{r}_{\rm p}) \\ \psi_{\sigma{\rm np}}(\mathbf{r}_\sigma, \mathbf{r}_{\rm n}, \mathbf{r}_{\rm p}) \end{pmatrix}, \tag{3}$$

where $\psi_{\rm np}$ is the wave-function of the two-body subsystem; $\psi_{\sigma{\rm np}}$ is the wave-function of the tree-body subsystem; and where $\mathbf{r}_{\rm n}$, $\mathbf{r}_{\rm p}$, $\mathbf{r}_\sigma$ and are the coordinates of the neutron, the proton, and the sigma-meson.

Correspondingly, the Hamiltonian is a matrix,

$$H = \begin{pmatrix} K_{\rm n} + K_{\rm p} & W \\ W & K_{\rm n} + K_{\rm p} + K_\sigma + m_\sigma \end{pmatrix}, \tag{4}$$

where $K_{\rm n}$, $K_{\rm p}$, K_σ are the kinetic energy operators for the neutron, the proton, and the sigma-meson; W is the coupling operator (to be introduced later); and m_σ is the mass of the sigma-meson.

It is of advantage to introduce relative Jacobi coordinates,

$$\mathbf{r}_{\rm np} = \mathbf{r}_{\rm p} - \mathbf{r}_{\rm n}, \quad \mathbf{r}_{\sigma{\rm np}} = \frac{m_{\rm n}\mathbf{r}_{\rm n} + m_{\rm p}\mathbf{r}_{\rm p}}{m_{\rm n} + m_{\rm p}} - \mathbf{r}_\sigma, \tag{5}$$

with the corresponding relative kinetic energy operators,

$$K_{\rm np} = -\frac{\hbar^2}{2\mu_{\rm np}}\frac{\partial^2}{\partial \mathbf{r}_{\rm np}^2}, \quad K_{\sigma{\rm np}} = -\frac{\hbar^2}{2\mu_{\sigma{\rm np}}}\frac{\partial^2}{\partial \mathbf{r}_{\sigma{\rm np}}^2}, \tag{6}$$

were the reduced masses are given as

$$\mu_{\rm np} = \frac{m_{\rm n} m_{\rm p}}{m_{\rm n} + m_{\rm p}}, \quad \mu_{\sigma{\rm np}} = \frac{m_\sigma (m_{\rm n} + m_{\rm p})}{m_\sigma + m_{\rm n} + m_{\rm p}}. \tag{7}$$

In the center-of-mass system the Hamiltonian is then given as

$$H = \begin{pmatrix} K_{\rm np} & W \\ W & K_{\rm np} + K_{\sigma{\rm np}} + m_\sigma \end{pmatrix}, \tag{8}$$

with the corresponding Schrodinger equation,

$$\begin{pmatrix} K_{\rm np} & W \\ W & K_{\rm np} + K_{\sigma{\rm np}} + m_\sigma \end{pmatrix} \begin{pmatrix} \psi_{\rm np}(\mathbf{r}_{\rm np}) \\ \psi_{\sigma pn}(\mathbf{r}_{\rm np}, \mathbf{r}_{\sigma{\rm np}}) \end{pmatrix} = E \begin{pmatrix} \psi_{pn}(\mathbf{r}_{\rm np}) \\ \psi_{\sigma pn}(\mathbf{r}_{\rm np}, \mathbf{r}_{\sigma{\rm np}}) \end{pmatrix}. \tag{9}$$

The coupling term for a scalar meson can be introduced in the integral form as

$$\langle \psi_{\rm np} \mid W \mid \psi_{\sigma{\rm np}} \rangle = \int d^3 r_{\rm np} d^3 r_{\sigma{\rm np}} \psi^*_{np}(\mathbf{r}_{\rm np}) W(\mathbf{r}_{\rm np}, \mathbf{r}_{\sigma{\rm np}}) \psi_{\sigma{\rm np}}(\mathbf{r}_{\rm np}, \mathbf{r}_{\sigma{\rm np}}). \tag{10}$$

One can assume that the nucleons themselves are already "dressed" with mesons and that the W-operator only accounts for the "extra" mesons generated due to the presence of another nucleon. The kernel $W(\mathbf{r}_{\rm np}, \mathbf{r}_{\sigma{\rm np}})$ then has to be of short range and has to vanish when either of the three particles is at larger distances. One of the simplest form is a Gaussian,

$$W(\mathbf{r}_{\rm np}, \mathbf{r}_{\sigma{\rm np}}) = S_\sigma \exp\left(-\frac{\mathbf{r}^2_{\rm np} + \mathbf{r}^2_{\sigma{\rm np}}}{b^2_\sigma} \right), \tag{11}$$

where the strength S_σ and the range b_σ are the parameters of the model. With this form there are two parameters per meson. The full model should presumably include π, σ, ρ, and ω mesons. That would make in total only eight parameters for all the traditional few-nucleon forces: central, tensor, spin-orbit, and three-body.

The coupled Schrodinger equation (9) can be solved numerically using the correlated Gaussian method described in the next section.

3 Correlated Gaussian Method for Coupled Few-Body Systems

In the correlated Gaussian method [11,12] the wave-function of a few-body quantum system is represented as a linear combination of correlated Gaussians,

$$e^{-\mathbf{r}^{\rm T} A \mathbf{r}} \equiv \exp\left(-\sum_{i,j=1}^{n} A_{ij} \mathbf{r}_i \cdot \mathbf{r}_j \right), \tag{12}$$

where $\mathbf{r} = \left(\mathbf{r}_1\ \mathbf{r}_2\ \ldots\ \mathbf{r}_n\right)^{\rm T}$ is a column-vector size-n set of the coordinates of the system; A is the matrix of parameters; and $\mathbf{r}_i \cdot \mathbf{r}_j$ signifies the scalar product of the two coordinates.

For the three-body σnp-subsystem the set $\mathbf{r}^{(\sigma)}$ of the center-of-mass coordinates is a two-component structure,

$$\mathbf{r}^{(\sigma)} = \begin{pmatrix} \mathbf{r}_{\rm np} \\ \mathbf{r}_{\sigma{\rm np}} \end{pmatrix}, \tag{13}$$

and the corresponding matrix A_σ is a two-times-two matrix. For the two-body np-subsystem the set $\mathbf{r}^{({\rm d})}$ of the center-of-mass coordinates is a simply a one-component structure,

$$\mathbf{r}^{({\rm d})} = \left(\mathbf{r}_{\rm np}\right), \tag{14}$$

and the corresponding matrix $A^{({\rm d})}$ is a one-times-one matrix. Despite the unit dimension we shall keep the matrix notation for consistency.

Now the wave-functions of the two subsystems are represented as

$$\begin{aligned} \psi_{\rm np}(\mathbf{r}^{({\rm d})}) &= \sum_{i=1}^{n^{({\rm d})}} c_i^{({\rm d})} e^{-\mathbf{r}^{({\rm d})\rm T} A_i^{({\rm d})} \mathbf{r}^{({\rm d})}} \equiv \sum_{i=1}^{n^{({\rm d})}} c_i^{({\rm d})} \langle \mathbf{r}^{({\rm d})} \mid A_i^{({\rm d})} \rangle\ , \\ \psi_{\sigma{\rm np}}(\mathbf{r}^{(\sigma)}) &= \sum_{j=1}^{n^{(\sigma)}} c_j^{(\sigma)} e^{-\mathbf{r}^{(\sigma)\rm T} A_j^{(\sigma)} \mathbf{r}^{(\sigma)}} \equiv \sum_{j=1}^{n^{(\sigma)}} c_j^{(\sigma)} \langle \mathbf{r}^{(\sigma)} \mid A_j^{(\sigma)} \rangle, \end{aligned} \tag{15}$$

where $n^{(\mathrm{d})}$ and $n^{(\sigma)}$ are the number of Gaussians in the subsystems, and where

$$\{c_i^{(\mathrm{d})}, c_j^{(\sigma)}, A_i^{(\mathrm{d})}, A_j^{(\sigma)}\}$$

are variational parameters. The non-linear parameters $\{A_i^{(\mathrm{d})}, A_j^{(\sigma)}\}$ are chosen stochastically while the linear parameters $c \doteq \{c_i^{(\mathrm{d})}, c_j^{(\sigma)}\}$ are obtained by solving the generalized eigenvalue problem,

$$\mathcal{H}c = E\mathcal{N}c, \tag{16}$$

where the matrices $\mathcal{N}$ and $\mathcal{H}$ are the overlap and the Hamiltonian matrix in the Gaussian representation (15). The matrices have the following two-times-two block structure,

$$\mathcal{H} = \begin{pmatrix} \left\langle A_i^{(\mathrm{d})} \mid K_{\mathrm{np}} \mid A_{i'}^{(\mathrm{d})} \right\rangle & \left\langle A_i^{(\mathrm{d})} \mid W \mid A_j^{(\sigma)} \right\rangle \\ \left\langle A_j^{(\sigma)} \mid W \mid A_i^{(\mathrm{d})} \right\rangle & \left\langle A_j^{(\sigma)} \mid K_{\mathrm{np}} + K_{\sigma\mathrm{np}} + m_\sigma \mid A_{j'}^{(\sigma)} \right\rangle \end{pmatrix}, \tag{17}$$

$$\mathcal{N} = \begin{pmatrix} \left\langle A_i^{(\mathrm{d})} \mid A_{i'}^{(\mathrm{d})} \right\rangle & 0 \\ 0 & \left\langle A_j^{(\sigma)} \mid A_{j'}^{(\sigma)} \right\rangle \end{pmatrix}, \tag{18}$$

where $i, i' = 1, \ldots, n^{(\mathrm{d})}$ and $j, j' = 1, \ldots, n^{(\sigma)}$.

One of the advantages of the correlated Gaussian method is that the matrix elements of the matrices $\mathcal{N}$ and $\mathcal{H}$ are analytic [13]. The cross terms are zero for all operators X except for the coupling operator W,

$$\langle A_i^{(\mathrm{d})} \mid X \mid A_j^{(\sigma)} \rangle = 0. \tag{19}$$

The overlap is given as

$$\langle A \mid A' \rangle = \left(\frac{\pi^{\mathrm{size}(A)}}{\det(A + A')} \right)^{\frac{3}{2}}. \tag{20}$$

The matrix element of the kinetic energy operator is given as

$$\langle A \mid -\frac{\partial}{\partial \mathbf{r}} K \frac{\partial}{\partial \mathbf{r}^{\mathrm{T}}} \mid A' \rangle = 6 \langle A \mid A' \rangle \operatorname{trace}\left(A K A' (A + A')^{-1} \right), \tag{21}$$

where the matrix K for the σnp-subsystem is given as

$$K^{(\sigma)} = \begin{pmatrix} \frac{\hbar^2}{2\mu_{\mathrm{np}}} & 0 \\ 0 & \frac{\hbar^2}{2\mu_{\sigma\mathrm{np}}} \end{pmatrix}, \tag{22}$$

and for the np-subsystem as

$$K^{(\mathrm{d})} = \begin{pmatrix} \frac{\hbar^2}{2\mu_{\mathrm{np}}} \end{pmatrix}. \tag{23}$$

The matrix element of the coupling operator (11) is given as

$$\langle A^{(\mathrm{d})} \mid W \mid A^{(\sigma)} \rangle = S_\sigma \langle \tilde{A} \mid A^{(\sigma)} \rangle, \tag{24}$$

where the matrix $\tilde{A}$ is given as

$$\tilde{A} = \begin{pmatrix} A^{(\mathrm{d})} + \frac{1}{b_\sigma^2} & 0 \\ 0 & \frac{1}{b_\sigma^2} \end{pmatrix}. \tag{25}$$

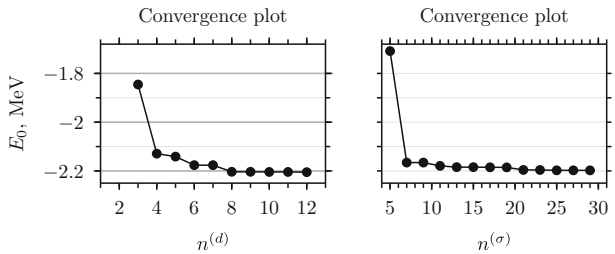

Fig. 1 Left: the deuteron ground-state energy, E_0, calculated with $n^{(d)}$ Gaussians in the two-body subsystem and 80 Gaussians in the three-body subsystem. Right: the deuteron ground-state energy, E_0, calculated with 25 Gaussians in the two-body subsystem and $n^{(\sigma)}$ Gaussians in the three-body subsystem

The generalized eigenvalue problem (16) is solved using the standard algorithm. First the symmetric positive-definite matrix $\mathcal{N}$ is Cholesky-factorized into a symmetric product, $\mathcal{N} = LL^{\mathrm{T}}$, where L is a lower-triangular matrix. The generalized eigenproblem (16) is then transformed into an ordinary symmetric eigenproblem,

$$\left(L^{-1}\mathcal{H}L^{-\mathrm{T}}\right)\left(L^{\mathrm{T}}c\right) = E\left(L^{\mathrm{T}}c\right) \tag{26}$$

The matrix $\left(L^{-1}\mathcal{H}L^{-\mathrm{T}}\right)$ is then diagonalized by any of the available diagonalization methods like the Jacobi eigenvalue algorithm.

Correlated Gaussians are naturally suited for bound state calculations as they vanish at large distances. Notwithstanding, they can also be used for continuum spectrum calculations. In particular, strength functions in the continuum can be calculated by placing the quantum system in an artificial trap, where continuum spectrum becomes discretized [14]. Cleverly chosen strength functions, calculated in the trap, can reveal resonances in the continuum [14]. Very narrow resonances can be investigated using the trap-variation (stabilization) method [12,14] or the complex scaling method [12]. Scattering problems can be solved using confining potential method [12], the Kohn variational method [12], or the resonating-group method [15].

4 Results

Given the meson mass, m_σ, the model has two free parameters: the strength, S_σ, and the range, b_σ, of the coupling operator (11). It turns out that for any $m_\sigma \in [100, 800]$ MeV it is possible to tune the parameters S_σ and b_σ such that the binding energy and the charge radius of the resulting deuteron are reasonable.

For illustration we assume m_σ=500 MeV similar to relativistic mean-field models [10]. With $m_\sigma = 500$ MeV and $m_\mathrm{n} = m_\mathrm{p} = 939$ MeV the parameters $b_\sigma = 3$ fm and $S_\sigma = 20.35$ MeV give the deuteron's ground-state energy $E_0 = -2.2$ MeV and the charge radius $R_c = 2.1$ fm which is close to the accepted values [16].

In this calculation we used low-discrepancy Van der Corput sampling strategy [17] for the non-linear parameters of the Gaussians. With this strategy the energy converges within 1% with about 10 Gaussians in the two-body subsystem and about 25 Gaussians in the three-body subsystem, as illustrated in Fig. 1. The final calculation has been done with $n^{(d)} = 25$ and $n^{(\sigma)} = 80$.

The radial wave-function of the deuteron in the two-body subsystem is shown in Fig. 2. For illustration the potential that produces the same wave-function via a radial Schrodinger equation is also shown. The potential is short-range and finite at the origin.

The contribution of the three-body σnp-subsystem to the norm of the total wave-function is only about 2%. This justifies the assumption that the two-meson contribution might be a small correction.

5 Conclusion

A nuclear model has been introduced where the nucleons interact by emitting and absorbing mesons which are treated explicitly. A nucleus in this model exists in a quantum superposition of states with increasing number of generated mesons.

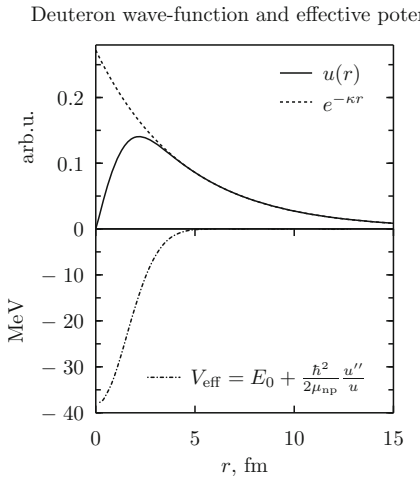

Fig. 2 Top: the radial wave-function, $u(r) = r\psi_{\rm np}(r)$, of the neutron-proton subsystem together with its asymptotic form, $\exp(-\kappa r)$, where $\kappa = \sqrt{2\mu_{\rm np}|E_0|/\hbar^2}$; bottom: the effective potential that produces the same radial wave-function as in the top figure

The model has been applied to the deuteron—in the model's simplest, one sigma-meson, incarnation—where the deuteron is a superposition of a two-body neutron-proton state and a three-body neutron-proton-sigma state. The model is able to produce a bound deuteron with very reasonable values of the binding energy and the charge radius.

The anticipated advantages of the model, compared to the phenomenological potential models, are the reduced number of parameters, natural inclusion of few-body forces, and natural inclusion of mesonic physics.

The next step in the development of the model could be inclusion of pions.

6 Appendix

6.1 Stochastic Sampling of Gaussian Parameters

The Gaussians can be parameterized in the form

$$\langle \mathbf{r} \mid A \rangle = \exp\left(- \sum_{i<j=1}^{N} \left(\frac{\mathbf{r}_i - \mathbf{r}_j}{b_{ij}} \right)^2 \right) \equiv \exp\left(-\mathbf{r}^{\rm T} A \mathbf{r} \right), \tag{27}$$

where $\mathbf{r}_i$ is the coordinate of the i-th particle and the matrix A is given as

$$A = \sum_{i<j=1}^{n} \frac{w_{ij} w_{ij}^{\rm T}}{b_{ij}^2}, \tag{28}$$

where the column-vectors w_{ij} are defined through the equation

$$\mathbf{r}_i - \mathbf{r}_j = w_{ij}^{\rm T} \mathbf{r}. \tag{29}$$

In the laboratory frame $\mathbf{r} = \left(\mathbf{r}_1 \ \mathbf{r}_2 \ \ldots \ \mathbf{r}_N \right)^{\rm T}$ and the w_{ij} are given for a two-body system as

$$w_{12} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{30}$$

and for a three-body system as

$$w_{12} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \quad w_{13} = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad w_{23} = \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}. \tag{31}$$

Under a coordinate transformation $\mathbf{r} \rightarrow J\mathbf{r}$ the column-vectors w_{ij} transform as $w_{ij} \rightarrow U^{\mathrm{T}} w_{ij}$ where $U = J^{-1}$.
The range parameters b_{ij} of the Gaussians are chosen stochastically from the exponential distribution,

$$b_{ij} = -\ln(u) b, \tag{32}$$

where the quasi-random number $u \in]0, 1[$ is taken from a Van der Corput sequence [17] with the scale $b = 3$ fm. Separate sequences with different prime bases are used for each ij-combination.

6.2 Charge Radius

We define the charge radius, R_c, of an N-body system as

$$R_c^2 = \sum_{i=1}^{N} Z_i \langle \mathbf{r}_i^2 \rangle = \sum_{i=1}^{N} Z_i \langle \mathbf{r}^{\mathrm{T}} w_i w_i^{\mathrm{T}} \mathbf{r} \rangle, \tag{33}$$

where the summation goes over the bodies in the system; Z_i is the charge of the body in unit charges; $\mathbf{r}_i$ is the coordinate of the body (in the center-of-mass frame); the brackets $\langle\rangle$ signify the expectation value in the given state of the system; and the column-vector w_i is defined via the formula

$$\mathbf{r}_i = w_i^{\mathrm{T}} \mathbf{r}. \tag{34}$$

In the laboratory frame, for a two-body system

$$w_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad w_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{35}$$

and for a three-body system

$$w_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, w_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, w_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{36}$$

Under a coordinate transformation $\mathbf{r} \rightarrow J\mathbf{r}$ the column-vector w_i transforms with the inverse matrix $U = J^{-1}$ as $w_i \rightarrow U^{\mathrm{T}} w_i$ (see Sect. 6.3 for a transformation to the center-of-mass frame).
Now the matrix element in (33) between two Gaussians is given as [13],

$$\left\langle A \mid \mathbf{r}^{\mathrm{T}} w_i w_i^{\mathrm{T}} \mathbf{r} \mid A' \right\rangle = \frac{3}{2} w_i^{\mathrm{T}} (A + A')^{-1} w_i \left\langle A \mid A' \right\rangle. \tag{37}$$

6.3 Coordinate Transformations

Under a linear coordinate transformation to a new set of coordinates,

$$\mathbf{r} \rightarrow \mathbf{x} = J\mathbf{r}, \tag{38}$$

the matrix elements with correlated Gaussians preserve their mathematical form as long as the determinant of the transformation matrix J equals one (otherwise they have to be divided by the determinant), and as long as

one makes the corresponding transformations of the related matrices and column-vectors: the kinetic energy matrix transforms as[1]

$$K \to J K J^{\mathrm{T}}, \tag{40}$$

and the w_i (and w_{ij}) column-vectors transform as[2]

$$w_i \to U^{\mathrm{T}} w_i, \tag{42}$$

where $U = J^{-1}$.
One practical set of coordinates are the Jacobi coordinates defined as

$$\mathbf{x}_{i<N} = \frac{\sum_{k=1}^{i} m_k \mathbf{r}_k}{\sum_{k=1}^{i} m_k} - \mathbf{r}_{i+1} \ , \ \mathbf{x}_N = \frac{\sum_{k=1}^{N} m_k \mathbf{r}_k}{\sum_{k=1}^{N} m_k} \ , \tag{43}$$

where the last coordinate, $\mathbf{x}_N$, is the center-of-mass coordinate that can be omitted if no external forces are acting on the system. This is equivalent to simply discarding the last row of the J matrix and the last column of the U matrix.

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[1] Which follows from the identity (with implicit summation notation),

$$\frac{\partial}{\partial \mathbf{r}_i} K_{ij} \frac{\partial}{\partial \mathbf{r}_j} = \frac{\partial}{\partial \mathbf{x}_k} \frac{\partial \mathbf{x}_k}{\partial \mathbf{r}_i} K_{ij} \frac{\partial}{\partial \mathbf{x}_l} \frac{\partial \mathbf{x}_l}{\partial \mathbf{r}_j} = \frac{\partial}{\partial \mathbf{x}_k} J_{ki} K_{ij} J_{lj} \frac{\partial}{\partial \mathbf{x}_l}. \tag{39}$$

[2] Which follows from the identity

$$w_i^{\mathrm{T}} \mathbf{r} = w_i^{\mathrm{T}} U \mathbf{x} = (U^{\mathrm{T}} w_i)^{\mathrm{T}} \mathbf{x}. \tag{41}$$