The few-body problem in terms of correlated gaussians

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Abstract

In their textbook, Suzuki and Varga [Y. Suzuki and K. Varga, Stochastic Variational Approach to Quantum-Mechanical Few-Body Problems (Springer, Berlin, 1998)] present the stochastic variational method in a very exhaustive way. In this framework, the so-called correlated gaussian bases are often employed. General formulae for the matrix elements of various operators can be found in the textbook. However the Fourier transform of correlated gaussians and their application to the management of a relativistic kinetic energy operator are missing and cannot be found in the literature. In this paper we present these interesting formulae. We give also a derivation for new formulations concerning central potentials; the corresponding formulae are more efficient numerically than those presented in the textbook.

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I. INTRODUCTION

There exist several different technical methods to solve the few-body problem with accuracy: Monte Carlo calculations [1], Faddeev and Yakubovsky treatments [2], hyperspherical formalism [3], expansion on various types of orthogonal [4], or non orthogonal bases [5]. Each techniques shows specific advantages and drawbacks. Among others, the stochastic variational method is especially attractive. It relies on expansion of the wave function in term of gaussian type functions. The stochastic algorithm allows to consider very large bases with a minimum of variational effort. The drawback of this method is the non orthogonality of basis wave functions with the possibility of appearance of spurious states due to overcompleteness; if this last inconvenient is overcome, using non orthogonal bases is not really a problem. The generalized eigenvalue problem arising in this case is well under control nowadays. The great advantage of using gaussian type functions is the rapid convergence and, above all, the possibility to compute the resulting matrix elements with analytical expressions most of time.

The stochastic variational method is described in full details in the remarkable textbook by Y. Suzuki and K. Varga [5], where most important and fundamental formulae are derived. This very complete work will be refered as SV throughout this paper, and all subsequent references can be found in it.

However, working on other projects, we were faced to the necessity to use some particularly important matrix elements that are not found in the exhaustive SV text-book. In particular, the Fourier transform of the correlated gaussians and the matrix elements of a relativistic kinetic energy operator are dramatically missing. In this paper, we want to complete SV with important formulæ that are of crucial importance for some applications. Besides the relativistic kinetic energy, we derive also new expressions for the matrix elements of central potentials. These expressions are simpler and more efficient numerically than those given in SV. We also report them here.

To achieve some unity, to precise our notations and to have a self-contained paper, we will also present below some formulæ already present in SV. In this case we give the references where they can be found in this work. We will derive formulæs for the case of one spatial coordinate ($L^2$ for spatial coordinates), the spatial part of the wave functions. Moreover, the non-natural parity states are very difficult to handle in correlated bases (this is possible but the expressions are much more involved) and, in the following, we just study natural parity (i.e spatial parity equal to $(-1)^L$) states.

The paper is organized as follows. We first describe the systems under consideration (intrinsic coordinates, definition of correlated gaussians and their generating functions). Then, we give the matrix elements for the overlap, the non-relativistic kinetic energy and a first expression for central potentials. Exception for special points, most of these formulæs can be found in SV. Lastly, the novelties concern new expressions for central potentials, the Fourier transform of correlated gaussians and its application to relativistic kinetic energy.
II. THE SYSTEM UNDER CONSIDERATION

The stochastic variational method can be applied to systems composed of more than one particle up to around ten particles. Let us denote by \( N + 1 \) the number of particles \((N \geq 1)\). The particle \( i \) is located at \( P_i \), so that the position vector relative to some origin \( O \) is \( OP_i = r_i \), and has a corresponding conjugate momentum \( p_i \). Since we are concerned only with spatial degrees of freedom, we ignore the color, isospin and spin variables.

It is interesting to introduce the center of mass coordinate \( R_{cm} = x_{N+1} \) and the corresponding total momentum \( P = \pi_{N+1} \). The intrinsic description is expressed in term of internal coordinates. There exist different possible choices depending upon the nature of the studied systems. Here, we are concerned only with the Jacobi coordinates.

A. Jacobi coordinates

In order to simplify the notations, let us note \( m_{12...i} = m_1 + m_2 + \ldots + m_i \) and \( G_i \) the center of mass of the first \( i \) particles: \( OG_i = (m_1 r_1 + m_2 r_2 + \ldots + m_i r_i) / m_{12...i} \).

The Jacobi coordinate \( x_i \) is defined as the position of the particle \( i + 1 \) relative to the center of mass \( G_i \) of the previous particles. Explicitly

\[
    x_i = OG_i - r_{i+1}.
\]

There are obviously \( N \) Jacobi coordinates \( x_i \) \((i \leq N)\) corresponding to intrinsic coordinates and the special vector \( x_{N+1} \) corresponds, as already mentioned, to the center of mass coordinate for the system (this vector has a physical meaning for particles with non vanishing masses; for the case of null mass particles, a way to get rid of this problem is to employ a relativistic kinetic energy, as explained in section VIII).

It is important to express the Jacobi coordinates in terms of the original position vectors

\[
    x_i = \sum_{j=1}^{N+1} U_{ij} r_j.
\]

It is easy to calculate, from definition (1), the value of the elements \( U_{ij} \):

\[
    U_{ij} = \frac{m_j}{m_{12...i}} \quad \text{if} \quad j \leq i,
\]

\[
    U_{ii+1} = -1,
\]

\[
    U_{ij} = 0 \quad \text{if} \quad j > i + 1.
\]

The inversion of relation (2) is often useful

\[
    r_i = \sum_{j=1}^{N+1} (U^{-1})_{ij} x_j.
\]

It is a matter of simple calculation to check that the matrix elements of the inverse matrix are given by:

\[
    (U^{-1})_{kl} = \frac{m_{l+1}}{m_{12...l+1}} k \leq l \leq N,
\]

\[
    (U^{-1})_{l+1,l} = -\frac{m_{l+2}}{m_{12...l+1}} l \leq N,
\]

\[
    (U^{-1})_{kl} = 0 \quad k > l + 1,
\]

\[
    (U^{-1})_{k,N+1} = 1 \quad \forall k.
\]

The conjugate momentum for variable \( x_i \) is denoted \( \pi_i = -i \partial / \partial x_i \) \((h = 1)\) and must fulfill the conditions \([x_i, \pi_j] = i \delta_{ij} \delta_{kl} \). It is easy to check that the relations corresponding to Eqs. (2)-(4) write

\[
    \pi_i = \sum_{j=1}^{N+1} (U^{-1})_{ji} p_j,
\]

\[
    p_i = \sum_{j=1}^{N+1} U_{ij} \pi_j.
\]

With this definition, the total momentum \( P = p_1 + p_2 + \ldots + p_{N+1} \) is just \( \pi_{N+1} \).

B. Correlated gaussians

In the stochastic variational method, the wave function for the system is expanded on gaussian type functions. There exist several different types of such basis states. Here we are concerned only with the so-called “correlated gaussians”. The space function is expressed in terms of the Jacobi coordinates.

The simplest version is a function that is a product of separate gaussian function for each Jacobi coordinate. In this case the calculations are very easy, but the convergence is slow, and, moreover, the available Hilbert space is enlarged and the convergence is accelerated.

To deal with a non vanishing total angular momentum, one must introduce spherical harmonics somehow or other. The most elegant manner is to use a single solid harmonic \( Y_{LM}(v) = \nu^L Y_{LM}(\hat{v}) \). To achieve some symmetry, and also to have more variational parameters at our disposal, the argument of the solid harmonic is the most general linear combination of the Jacobi coordinates: \( \sum_{i,j=1}^{N} A_{ij} x_i \cdot x_j \). The matrix \( A \) must be symmetric \((A = A)\) and positive definite. Obviously, the Hilbert space is enlarged and the convergence is accelerated.

In order to simplify the notations, let us introduce a “super-vector” \( \tilde{x} = (x_1, x_2, \ldots, x_N) \) and write the coefficients of linear combinations as a “line (or column) matrix”, i.e \( \tilde{u} = (u_1, u_2, \ldots, u_n) \). This allows to shorten
the expressions using the usual matrix operations. For example (the presence of the symbol \( \cdot \) deals with a spatial scalar product, while the absence deals only with a linear combination)

\[
\sum_{i,j=1}^{N} A_{ij} x_i \cdot x_j = \tilde{x} \cdot A x,
\]

\[
\sum_{i=1}^{N} u_i x_i = \tilde{u} x.
\]

(8)

With those definitions, the most general correlated gaussian is given by (note a slight difference with SV notations; their matrix \( A \) is twice ours and moreover \( N \) is the number of Jacobi coordinates while SV consider it as the number of particles)

\[
f_{KLM}(u, A; x) = \exp(-\tilde{x} \cdot A x) |\tilde{u} x|^{2K} Y_{LM}(\tilde{u} x).
\]

(9)

The correlated gaussian represents the basis state in coordinate representation \( f_{KLM}(u, A; x) = (x|\psi_{KLM}(u, A)) \). Thus each basis state is described by \( N(N + 1)/2 \) for the matrix \( A \) and \( N \) for the vector \( u \). This prescription is only able to deal with natural parity states. The term \( |\tilde{u} x|^{2K} \) is introduced for generality and to treat with more accuracy potentials with specific singular features. However, it complicates a lot the resulting expressions. It is often more convenient (except when the potential is so singular that the resulting integrals diverge) to keep in the calculation the correlated gaussians restricted to \( K = 0 \), including more basis states to compensate a slower convergence. The even simplest version corresponds to a diagonal \( A \) matrix.

C. Matrix elements and generating functions

We are interested in the calculation of the matrix elements for some operator \( \hat{O} \) on the correlated gaussians, namely \( \langle \psi_{K'LM'}(u', A')|\hat{O}|\psi_{KLM}(u, A) \rangle \). The critical point in the computation of such element is to manage the difficulties due to the presence of the solid harmonics. An artful way to deal with them is to use the generating functions for the correlated gaussians. Since the technical details can be found in SV, we just recall below the most important results and let the reader have a look on SV (in section 6.3) for rigorous proofs.

Let us define the functions

\[
g(s, A; x) = \exp(-\tilde{x} \cdot A x + \tilde{s} \cdot x)
\]

(10)

where \( s \) is an arbitrary super-vector, \( \tilde{s} = (s_1, s_2, \ldots, s_N) \), and, as usual \( \tilde{s} \cdot x = \sum_{i=1}^{N} s_i \cdot x_i \).

The \( g \) functions are called the generating functions for the correlated gaussians since one has

\[
f_{KLM}(u, A; x) = \frac{1}{B_{KL}} \times \int \! d\tilde{e} Y_{LM}(\tilde{e}) \left( \frac{\partial^2 K + L}{\partial \lambda^2} g(\lambda e u, A; x) \right)_{\lambda=0,|e|=1}
\]

where the geometrical coefficient \( B_{KL} \) is defined as

\[
B_{KL} = \frac{4\pi(2K + L)!}{2^K K!(2K + 2L + 1)!!}.
\]

(11)

In Eq. (11), the super-vector \( s = \lambda e u \) must be understood with all its components proportional to the same three vector \( e \), namely \( s_i = \lambda u_i e \).

Using Eq. (11) in the expression of the searched matrix element leads to

\[
\langle \psi_{K'LM'}(u', A')|O|\psi_{KLM}(u, A) \rangle
= \frac{1}{B_{K'LM'}B_{KL}} \int \! d\tilde{e} \tilde{e}' Y_{LM}(\tilde{e}) Y_{LM}^*(\tilde{e}')
\]

\[
\times \left( \frac{\partial^2 K' + L' + 2K + L}{\partial \lambda^2} \frac{\partial^2 K + L + 2K + L}{\partial \lambda^2} \right)_{\lambda=0,|e|=|e'|=1} \langle O \rangle_{\lambda=0,|e|=|e'|=1}.
\]

(13)

with the matrix element between the generating function

\[
\langle O \rangle = \langle g(\lambda e' u', A'; x)|O|g(\lambda e u, A; x) \rangle
\]

(14)

The matrix element that is left for computation is now between the generating functions, the form of which is much simpler.

In the rest of the paper, we focus our study on operators that are scalar for spatial coordinates, so that the only non vanishing elements are those with \( L = L' \), and \( M = M' \). Moreover, the matrix elements do not depend on the magnetic quantum number \( M \).

III. OVERLAP

The overlap between basis states \( N_{K'KL} = \langle \psi_{K'LM'}(u', A')|\psi_{KLM}(u, A) \rangle \) is a crucial ingredient in the equation of motion. Since the basis states are non orthogonal, there is no reason that such an element is diagonal.

As already mentioned, it is easier to calculate first the elements for the generating functions. The technics is always the same; we first diagonalize the matrix \( A \) and change the integration variables to the eigenvectors of \( A \). More details are presented in SV, and we will develop more deeply this technics later on. Explicitly, one finds (see SV, Table 7.1 page 124):

\[
\langle g(s', A'; x)|g(s, A; x) \rangle = \left( \frac{\pi N}{|\det B|} \right)^{3/2} \exp \left( \frac{1}{4} \tilde{\theta} \cdot B^{-1} \tilde{v} \right) = M_0
\]

(15)
where

\[ B = A + A'; \quad v = s + s'. \]  

(16)

The overlap is obtained introducing result (15) in the general formula (13). Since the variables \( \lambda, \lambda', e, e' \) appear only in \( v \), the term depending on \( \det B \) factorizes out the integral. The exponential is then expanded as a series in \( \lambda, \lambda', e, e' \). The derivation and integration are performed without difficulty. The final result is (SV, (A.6) page 248)

\[ \mathcal{N}_{K'KL} = \frac{(2K' + L)! (2K + L)!}{B_{K'L} B_{KL}} \left( \frac{\pi^N}{\det B} \right)^{3/2} \]

with the following complementary definitions

\[ q = \frac{1}{4} \tilde{u} B^{-1} u; \quad q' = \frac{1}{4} \tilde{u}' B^{-1} u'; \quad \rho = \frac{1}{2} \tilde{u}' B^{-1} u = \frac{1}{2} \tilde{u} B^{-1} u'. \]  

(18)

For the important peculiar case \( K' = K = 0 \), this formula simplifies a lot and we are left with (SV (A.7) page 249):

\[ \mathcal{N}_{00L} = \mathcal{N}_L = \frac{(2L + 1)!!}{4\pi} \left( \frac{\pi^N}{\det B} \right)^{3/2} \rho^L. \]  

(19)

IV. NON RELATIVISTIC KINETIC ENERGY

It is well known that the use of Jacobi coordinates allows to share the total kinetic energy operator \( T = \sum_{i=1}^{N+1} p_i^2/(2m_i) \) into the kinetic energy of the system as a bulk \( T_{cm} = P^2/(2M) \) \((M = m_1 \ldots m_{N+1})\) and an intrinsic kinetic energy operator \( T_{NR} \) depending only on intrinsic momenta.

A simple calculation leads to the explicit expression

\[ T_{NR} = T - T_{cm} \]

\[ = \frac{1}{2} \sum_{i,j=1}^{N} \Lambda_{ij} \pi_i \cdot \pi_j - \frac{1}{2} \tilde{\pi} \cdot \Lambda \tilde{\pi} \]  

(20)

where the super-vector \( \tilde{\pi} = (\pi_1, \pi_2, \ldots, \pi_N) \) is introduced. The matrix \( \Lambda \) is symmetric and its general element writes

\[ \Lambda_{ij} = \sum_{k=1}^{N+1} U_{ik} U_{jk} \frac{1}{m_k}. \]  

(21)

The matrix elements of \( T_{NR} \) on correlated gaussians rely again on the expression of the elements on the generating functions. This calculation is a bit more complicated, but one can show that (see SV, Table 7.1 page 124):

\[ \langle g(s', A'; x)|\tilde{\pi} \cdot \Lambda \tilde{\pi}|g(s, A; x)\rangle = \mathcal{M}_0 [6 \text{Tr}(AB^{-1}A') - \tilde{y} \cdot \Lambda \tilde{y}] \]  

(22)

where \( \mathcal{M}_0 \) is precisely the overlap expression (15), \( \text{Tr}(X) \) means the trace of the \( X \) matrix, and the super-vector \( y \) is given by

\[ y = A' B^{-1} s - AB^{-1} s'. \]  

(23)

It remains to insert result (22) into Eq. (13). The variables \( \lambda, \lambda', e, e' \) appear now still in the exponential part of \( \mathcal{M}_0 \) but also in \( \tilde{y} \cdot \Lambda \tilde{y} \) while the trace is independent of these. Fortunately, the new contribution is just a polynomial in term of these variables. Thus, developing the exponential as a series leads to a total contribution which is polynomial and which can be treated exactly in the same way as the overlap.

The final result is (see SV, (A.10) page 250)

\[ \langle \psi_{K'LM}(u', A')|\tilde{\pi} \cdot \Lambda \tilde{\pi}|\psi_{KL}(u, A)\rangle = \frac{(2K' + L)! (2K + L)!}{B_{K'L} B_{KL}} \left( \frac{\pi^N}{\det B} \right)^{3/2} \]

\[ \times \sum_{k=0}^{\min(K,K')} B_{kL} \left[ R q q' \rho + P(K - k) q' \rho + P'(K' - k) q \rho + Q(2k + L) q q' \right] \frac{q^{K-k-1} q'^{K'-k-1} \rho^{2k+L-1}}{(K-k)! (K'-k)! (2k+L)!}. \]  

(24)

with the numbers \( P, P', Q, R \) defined by

\[ P = -\tilde{u} B^{-1} A' A' B^{-1} u; \quad P' = -\tilde{u}' B^{-1} A A B^{-1} u'; \quad Q = 2\tilde{u} B^{-1} A A' B^{-1} u; \quad R = 6 \text{Tr}(AB^{-1}A'). \]  

(25)

Again, the formula for the special case \( K = K' = 0 \) is
It is necessary to calculate the matrix elements of \( \delta \). The most general form of the potential is a sum of terms like a linear combination of Jacobi coordinates, so that the potential has a form \( V = \sum_{i<j} V_{ij} \) or two-body potentials. In the first situation, the potential has a form \( V = \sum_{i} V_i \) in this case, \( \Lambda_{ij} = (1/\mu_i) \delta_{ij} \).

### V. CENTRAL POTENTIALS: A FIRST EXPRESSION

In the most interesting cases, the potentials appearing in the few-body problem are either one-body potentials or two-body potentials. In the first situation, the potential has a form \( V = \sum_i V_i(r_i - R_{cm}) \) while the second situation the potential has a form \( V = \sum_{i<j} V_{ij}(r_i - r_j) \). This is the consequence of translational invariance. In both cases, the argument of any potential is a linear combination of Jacobi coordinates, so that the most general form of the potential is a sum of terms like \( V(\tilde{w} \cdot \mathbf{r}) \).

In this case, one can write generally

\[
\langle \psi | V(\tilde{w} \cdot \mathbf{r}) | \psi \rangle = \int V(r) \langle \psi | \delta^3(\tilde{w} \cdot \mathbf{r}) | \psi \rangle \, dr.
\]  

It is necessary to calculate the matrix elements of \( \delta(\tilde{w} \cdot \mathbf{r}) \) on the generating functions; these are given in SV Table 7.1 page 124.

However, we are interested here in central potentials that are also invariant under rotations; the argument of the potential must be now [\( \tilde{w} \cdot \mathbf{r} \)]. In this case, the equivalent expression of (29) needs a single integral

\[
\langle \psi | V(\tilde{w} \cdot \mathbf{r}) | \psi \rangle = \int V(r) \langle \psi | \delta(\tilde{w} \cdot \mathbf{r}) | \psi \rangle \, dr.
\]  

It is necessary to calculate the matrix elements of \( \delta(\tilde{w} \cdot \mathbf{r}) \) on the generating functions. They are not given in SV. It is possible to get them either directly by elementary integrations, or by the developing \( \delta^3(\tilde{w} \cdot \mathbf{r}) \) in spherical coordinates and integrating on angular variables. We find

\[
\langle g(s', A'; x) | \delta(\tilde{w} \cdot \mathbf{r}) | g(s, A; x) \rangle = \frac{4M_0}{\sqrt{\pi}} \times \frac{r^2}{(wB^{-1}w)^{3/2}} \int \left( \frac{r \tilde{w} B^{-1} \mathbf{v}}{w B^{-1}w} \right) \exp \left( -\frac{r^2 + (\tilde{w} B^{-1} \mathbf{v})^2}{4} \right)
\]  

where \( i_0(z) = \sinh(z)/z \) is a modified spherical Bessel function.

One must implement the element (31) into Eq. (13). For further convenience, we give here more information concerning this computation. Let us note \( c = 2/(wB^{-1}w) \). First, it is possible to remove the term \( \exp(-cr^2/2) \) and all terms depending on \( c \) only out of the derivation and, even, out of the integral. The terms containing the variables \( \lambda, \lambda', \mathbf{e} \cdot \mathbf{e}' \) are present in the exponential part of \( \mathcal{M}_0 \) which writes explicitly

\[
\mathcal{M}_0 \propto \exp(q^2 + q'\lambda^2 + \rho \lambda \lambda' \mathbf{e} \cdot \mathbf{e}').
\]  

These terms also appears in the variable \( z = (\tilde{w} B^{-1} \mathbf{v})/2 \). Let us introduce the numbers \( \gamma = c(\tilde{w} B^{-1}u)/2, \gamma' = c(\tilde{w} B^{-1}u')/2 \). The variable \( z \) now reduces to \( cz = \gamma \lambda \mathbf{e} + \gamma' \lambda' \mathbf{e}' \). Thus, the term \( i_0(c r | z) \) \( \exp(-cz^2/2) \) must also be included in the derivation term.

Using the fact that \( \exp(-s^2 + 2sx) \) is the generating function for Hermite polynomials \( H_n(x) \), it is possible to prove the interesting relation

\[
i_0(Bz) \exp(-Az^2) = \frac{\sqrt{A}}{B} \sum_{n=0}^{\infty} \frac{(A z^2)^n}{(2n + 1)!} H_{2n+1}(B/2\sqrt{A}).
\]  

The technics presented in SV consists in employing this formula to evaluate \( i_0(c r | z) \) \( \exp(-cz^2/2) \). Forgetting terms depending on \( c \) only, there appears a term depending on \( r: H_{2n+1}(r \sqrt{c}/2) / r \) and a term

\[
(c^2 z^2)^n = (\gamma^2 \lambda^2 + \gamma'^2 \lambda'^2 + 2\gamma\gamma' \lambda \lambda' \mathbf{e} \cdot \mathbf{e}').
\]  

which must be maintained in the derivation and which is expanded as a series. It is gathered with the series coming from exponential (32). After this grouping, the general monome of this series has the form \( \lambda^* \lambda'^* (\mathbf{e} \cdot \mathbf{e}')^t \). The derivation \( \partial^2 K+L / \partial \lambda^{2K+L} \) being taken for \( \lambda = 0 \) leads to a term \( (2K + L)! \delta_{2K+L,s} \); one has also a term \( (2K' + L)! \delta_{2K'+L,s'} \) coming from the derivation with respect to \( \lambda' \). Lastly, the term \( (\mathbf{e} \cdot \mathbf{e}')^t \) is expanded as (do not forget that \( |\mathbf{e}| = 1 = |\mathbf{e}'| \))

\[
(\mathbf{e} \cdot \mathbf{e}')^t = 4\pi \sum_{l m} \frac{t!}{(l-t)! (l+l+1)!} Y^*_{lm}(\hat{e}) Y_{lm}(\hat{e}'),
\]  

and the integration over \( \hat{e} \) and \( \hat{e}' \) leads to a term \( B_{kL} \delta_{2k+L,t} \).
Lastly, the geometrical function $H$ is defined by
\[ H_{n,k}^{K,K',L}(x,x',y) = \sum_{r=0}^{K+K'+L-n} (-1)^r \frac{(K+K'+L-r)!}{(K+K'+L-n-r)!} G_{n,k,r}^{K,K',L}(x,x') \]
(43)

with function $H$ defined by
\[ H_{n,k}^{K,K',L}(x,x',y) = \sum_{r=0}^{K+K'+L-n} (-1)^r \frac{(K+K'+L-r)!}{(K+K'+L-n-r)!} G_{n,k,r}^{K,K',L}(x,x') \]
(43)

and
\[ G_{n,k,r}^{K,K',L}(x,x') = \sum_{s=0}^{K-k'} \sum_{s'=0}^{K'-k} x^s x'^{s'} \frac{1}{[r-s-s']!(2k+L+s+s'-r)!} \]
(44)

In this formula, the dynamical quantities $q, q', \rho$ have been defined in Eq. (18) for the overlap, while the new ones $c, \gamma, \gamma'$ are specific to the potential
\[ c = \frac{2}{\bar{w} B^{1/2}}; \quad \gamma = \frac{\bar{w} B^{-1} u}{\bar{w} B^{1/2}}; \quad \gamma' = \frac{\bar{w} B^{-1} u'}{\bar{w} B^{1/2}}. \]
(37)

The form of the potential appears explicitly through the following integral
\[ J(n, c) = \frac{1}{\sqrt{\pi(2n+1)!}} \int_0^{\infty} V(x) \frac{2}{e^{-x^2}} H_1(x) H_{2n+1}(x) dx. \]
(38)

Lastly, the geometrical function $F$ is defined as
\[ F_{p,p',l}^{n}(q,q',\rho,\gamma,\gamma') = n! \sum_{m,m'} (p-m)! (p'-m')! \gamma^{n+m-m'} \frac{\rho^{l-n+m-m'}}{(l-n+m+m')! 2^{m+m'} m! m'! (n-m-m')!}. \]
(39)

We tried to express this function in terms of hypergeometric functions, but without success (when no explicit bounds are indicated, the indices in the summations run on values that do not give integer negative values for the factorials).

The expression (36) has the nice property to allow easy checks. The bra-ket symmetry is trivial. For such a symmetry, $K \leftrightarrow K'$, $A \leftrightarrow A'$, $u \leftrightarrow u'$, $q \leftrightarrow q'$, $\gamma \leftrightarrow \gamma'$, while $B$, $\rho$ and $c$ remain unchanged. The symmetry follows from the property $F_{p,p',l}^{n}(q,q',\rho,\gamma,\gamma') = F_{p,p',l}^{n}(q',q,\rho,\gamma',\gamma)$. It is also easy to recover the overlap expression if we set $V(r) = 1$. In this case, due to the orthogonality of Hermite polynomials, one has $J(n,c)/c^n = 1$, $F_{p,p',l}^{n}(q,q',\rho,\gamma,\gamma') = \rho^n \rho''' \rho'/[p! p'! l!]$ and the overlap expression follows immediately.

As always, there is a great simplification in the special case $K = K' = 0$. Indeed, one has the simple expression (SV, (A.130) page 282)
\[ \langle \psi_{0LM} | V(\bar{w} x) | \psi_{0LM} \rangle = N_L L! \sum_{n=0}^{L} \frac{J(n,c)}{(L-n)!} \left( \frac{\gamma' \rho}{\rho c} \right)^n. \]
(40)

Here again, the overlap factorizes.

A small drawback in the formulae (36) and (40) is the presence of the Hermite polynomial $H_{2n+1}(x)$. One way to deal with it is the use of recursion formulae. However, the accuracy decreases with increasing $n$; moreover, closed expressions for $J(n,c)$ do not exist for various forms of potential $V(r)$. There is a way to get rid of these two difficulties.

We define new integrals:
\[ F_V(k, A) = \int_0^{\infty} V(u) u^k e^{-A u^2} du. \]
(41)

Indeed, a lot of closed expressions exist for various forms of potentials $V(u)$. Expanding the Hermite polynomials as a series, and rearranging the summations leads to a new expression for the matrix elements in terms of $F_V$ functions. This form is absent in SV.
Due to the property $G_{n,k,r}^{K,K',L}(x,x') = G_{n,k,r}^{K',K,L}(x',x)$ the hermiticity of the element is transparent.

For the special case $K = K' = 0$, this formula reduces to

$$\langle \psi_{0LM}(u', A') | V(|\tilde{w}x|) | \psi_{0LM}(u, A) \rangle = N_L 2c \sqrt{\frac{c}{2\pi}} L! \times \sum_{n=0}^{L} \frac{c_n^2}{(2n+2)!} \left( \frac{\gamma'}{\rho} \right)^n \left( 1 - \frac{\gamma'}{\rho} \right)^{L-n} . (45)$$

This formula needs essentially the same numerical effort than expression (40) but it is written in terms of a much more convenient integral.

VI. CENTRAL POTENTIALS: A NEW EXPRESSION

In this section we present new formulae for the matrix elements of a central potential; the corresponding expressions are more efficient for a numerical treatment.

Let us remark that the relationship (33) gives a link between $e,e'$ and the variable $z$. This opportunity allows to put the exponential (42) under the form

$$\exp(\bar{q}z^2 + \bar{q}'z^2 + \rho c^2 z^2/(2\gamma'))$$

with the new variables $\bar{q} = q - \rho\gamma/(2\gamma')$ and $\bar{q}' = q' - \rho\gamma'/(2\gamma)$.

One gathers the part of exponential depending upon $z$ with the other exponential depending upon $z$ into a single exponential which takes the form $\exp(-\bar{c}z^2/2)$ with the definition $\bar{c} = c(1 - \rho c/(\gamma\gamma'))$. We then treat the term $i\rho(c'z)$ $\exp(-\bar{c}z^2/2)$ with the already mentioned relation (33). The rest of the derivation is essentially similar to that of section V. The trick of gathering two exponentials into a single one allows to gain one expansion into a series; the price to pay is the use of renormalized dynamical quantities.

The final formula, which is absent in SV, looks like

$$\langle \psi_{K',LM}(u', A') | V(|\tilde{w}x|) | \psi_{KLM}(u, A) \rangle =$$

$$\frac{(2K' + L)! (2K + L)!}{B_{K'\cdot L} B_{K\cdot L}} \left( \frac{\alpha \pi}{\det B} \right)^2 \times$$

$$\sum_{n=0}^{\min(K,K')} \left( \frac{\alpha}{2c} \right)^n J(n, \alpha, c) \times$$

$$\times \sum_{k=0}^{2K + L} \frac{2^{2k + L}}{(2k + L)!} B_{K'\cdot L} F_{n,k}^{K,K',L}(\bar{q}, \bar{q}', \gamma, \gamma').$$

In this formula, the dynamical quantities $c, \gamma, \gamma'$ are identical to those defined in Eq. (37) while new quantities are necessary

$$\bar{q} = q - \frac{\rho\gamma}{2\gamma}; \quad \bar{q}' = q' - \frac{\rho\gamma'}{2\gamma}; \quad \alpha = 1 - \frac{\rho c}{\gamma\gamma'} . (48)$$

The form of the potential appears explicitly through an integral of new type

$$J(n, \alpha, c) = \frac{1}{\sqrt{\pi}(2n + 1)!} \times \int_0^\infty V(x) e^{-x^2} H_1(x) H_{2n+1}(x) \, dx . (49)$$

Lastly, the geometrical function $F$ is defined by

$$F_{n,k}^{K,K',L}(x,x',y,y') = n! \sum_{m=\max(k+L,n-K')}^{\min(n-k,K+L)} \frac{2^{K+L-m}}{(K + L - m)!} \times$$

$$\times \frac{1}{(K' - n + m)! (m - k - L)! (n - k - m)!} . (50)$$

Comparison between equivalent forms (46), given in SV, and (47), novelty of this paper, warrants some comments.

- They both have very similar aspect. The new form requires the calculations of 3 new quantities $\bar{q}, \bar{q}', \alpha$ and an integral $J(n, \alpha, c)$ instead of $J(n, c)$. But in doing this, the numerical effort is essentially the same. In contrast, the rest of the calculation is much more efficient under the new version; indeed the $F$ function depends on 4 variables instead of 5, it requires a single summation instead of a double and the general monomie needs one factorial less.

- The equivalence between both can be proved using the following very interesting relationship

$$\int_0^\infty \frac{1}{a(a^2 - 1)^2} \int_0^\infty f(y) e^{-y^2} H_1(y) H_{2L+1}(ay) \, dy =$$

$$\sum_{n=0}^{L} \left( \frac{2L + 1}{L - n} \right) \frac{(2L + 1)!}{(L-n)! (n+1)!} \times$$

$$\times \int_0^\infty f(y) e^{-y^2} H_1(y) H_{2n+1}(y) \, dy , (51)$$

valid for any function $f(y)$.

- The symmetry properties are more transparent in the SV version, but they can be proved as well in the new version. Once the equivalence between both is shown this point is of minor importance.

The new version is especially interesting in the peculiar case $K = K' = 0$ since the result writes

$$\langle \psi_{0LM}|V(|\tilde{w}x|)|\psi_{0LM} \rangle = N_L L! \left( \frac{\alpha}{1 - \alpha} \right)^L \alpha^{3/2} J(L, \alpha, c) . (52)$$

In this case, there is no summation at all!
To finish this part, let us derive the general formula expressed in terms of the \(F\) integral instead of the \(J\) integral. The calculation relies essentially on the techniques presented in section \(\S\). The result is

\[
\langle \psi_{K',LM}(u', A') V([\tilde{w} \tilde{x}]) \psi_{KLM}(u, A) \rangle = \\
\frac{4(2K'+L)! (2K+L)!}{\pi B_{K',L} B_{K,L}} \left( \frac{cn N}{2 \det B} \right)^{3/2} \\
\times \sum_{n=0}^{K+K'+L} \frac{\mathcal{F}_V(2n+2, c/2)}{(2n+1)!} \\
\times \sum_{k=0}^{\min(K, K')} \frac{2^{2k+L}}{(2k+L)!} B_{kL} G_{n,k}(\tilde{q}, \tilde{q}', \gamma, \gamma', c)
\]

(53)

with function \(G\) defined by

\[
G_{n,k}(\tilde{q}, \tilde{q}', \gamma, \gamma', c) = \\
\sum_{r=k+L}^{K'+L} \frac{\tilde{q}^{K-L-r} \tilde{q}'^{r} \gamma^{n-r} \gamma'^{2r-L}}{(K+L-r)! (r-k-L)!} M_{n,k,r} \left( \frac{\alpha \gamma^2}{2 \tilde{q}'} \right)
\]

(54)

and with

\[
M_{n,k,r}(z) = \sum_{s=\max(0,k+r-n)}^{K'+r-n} \frac{(s+n)!}{(K'+r-s-n)! (s+n-k-r)!} \frac{z^s}{s!}
\]

(55)

This formulation is also more efficient numerically than \[\text{[42]}\] for the same reasons as those explained above.

Application of this formula to the special case \(K = K' = 0\) leads exactly to the formula \[\text{[15]}\] got before and thus does not bring any novelty.

\textbf{VII. FOURIER TRANSFORM OF CORRELATED GAUSSIANS}

For a number of applications, it is useful to have the Fourier transform (FT) of correlated gaussians. This point is missing in SV and, to our knowledge, such an expression seems absent in the literature. In this section, we want to derive the corresponding relation.

The basic ingredient for this calculation is the FT of a correlated gaussian limited to one variable, namely the value of the integral

\[
(2\pi)^{-3/2} \int e^{-i\mathbf{q} \cdot \mathbf{x}} e^{-\alpha^2 r^2} r^{2K} \mathcal{Y}_{LM}(r) \, dr.
\]

(56)

The first thing to do is to use the traditional development of a plane wave in terms of spherical harmonics

\[
e^{-i\mathbf{q} \cdot \mathbf{x}} = 4\pi \sum_{m=-L}^{L} (-i)^l j_l(qr) Y_{lm}(\hat{r}) \text{ where } j_l(z) = \sqrt{\pi/(2z)} J_{l+1/2}(z)
\]

is the spherical Bessel function. Integration over angular \(\hat{r}\) variables leads to a \(\delta_{m,LM}\) factor which restricts the infinite summation to the single term \(l = L, m = M\). Apart from some constant factors that can be gathered outside the integral, we are left with a radial integral, which, after a trivial change of variable, can be put under the form

\[
\int_0^{\infty} e^{-x^2} x^{2K+L+3/2} J_{L+1/2}(q) \, dx = \frac{n!}{2 \sqrt{\pi}} e^{-\frac{1}{2} x^2} x^{L+1/2}.
\]

Fortunately, this integral is analytical and can be expressed in terms of generalized Laguerre polynomial \(L_n^\mu\). This miraculous formula can be found in Ref. \[\text{[7]}\] (formula (6.601) n 10, page 738): it writes (it can be obtained using the generating function of Laguerre polynomials expressed in term of Bessel functions \[\text{[2]}\])

\[
\int_0^{\infty} e^{-x^2} x^{2n+\mu+1} J_{\mu}(2\sqrt{x}) \, dx = \frac{n!}{2} e^{-x^2} x^{\mu/2} L_n^\mu(x).
\]

(57)

In this formula \(\mu\) is any real number \(> -1\) and \(n\) is a positive or null integer. The case \(n = 0\) is simpler due to the property \(L_0^0(z) = 1, \forall z\). We thus get the searched integral

\[
\frac{1}{(2\pi)^{3/2}} \int e^{-i\mathbf{q} \cdot \mathbf{x}} e^{-\alpha^2 x^2} x^{2K} \mathcal{Y}_{LM}(x) \, dx = \\
\frac{K!}{\alpha^{K L+1/2}} \left( \frac{q^2}{4\alpha} \right)^{L+1/2} e^{-q^2/(4\alpha)} \mathcal{Y}_{LM}(q).
\]

(58)

To get the formula corresponding to \(K = 0\), it is sufficient to replace in Eq. \[\text{[53]}\] the terms depending on \(K\) by 1, at the head of the right hand side expression.

To derive the general FT, we begin, for pedagogical reasons, with the special case \(K = 0\). Let us note

\[
h_{LM}(u; A; \mathbf{a}) = (2\pi)^{-3N/2} \int e^{-i\pi \cdot \mathbf{a} \cdot x} f_{0LM}(u; \mathbf{a}) \, dx
\]

\[
= (2\pi)^{-3N/2} \int e^{-i\mathbf{a} \cdot \mathbf{x}} x^{-i\mathbf{a} \cdot T D^{-1/2} \mathbf{z}} \mathcal{Y}_{LM}(\mathbf{u} T D^{-1/2} \mathbf{z}) \, dx = I.
\]

(59)

The matrix \(A\) is symmetric and thus can be diagonalized with an orthogonal matrix \(T : A = T D T\). Being positive definite, all the eigenvalues of the diagonal matrix \(D\) are positive, and there is no problem to build the square root \(D^{1/2}\) of this matrix. Instead of the original \(\mathbf{x}\) variables, it is wily to work with the new variables \(\mathbf{z} = D^{1/2} T \mathbf{x}\). At this stage, one has

\[
I = (2\pi)^{-3N/2} (\det A)^{-3/2} \times \\
\int d\mathbf{z} \exp(-\mathbf{z} \cdot \mathbf{z} - i\mathbf{\tilde{a}} \cdot T D^{-1/2} \mathbf{z}) \mathcal{Y}_{LM}(\mathbf{\tilde{u} T D^{-1/2} z}).
\]

(60)

In a second step, we change again from \(\mathbf{z}\) to new \(\mathbf{Z}\) variables with the help of an orthogonal matrix \(U : \mathbf{Z} = U \mathbf{z}\). The Jacobian of the transformation is unity, and, moreover, \(\mathbf{\tilde{z}} \cdot \mathbf{Z} = \mathbf{\tilde{Z}} \cdot \mathbf{Z}\). There is a large freedom in the choice of the \(U\) matrix. One can take this opportunity making a choice such that the argument of the solid harmonic is proportional to one of the new variables, let us say \(\mathbf{Z}_1\). Now, the integral takes the form:

\[
I = (2\pi)^{-3N/2} (\det A)^{-3/2} \times \\
\times \int d\mathbf{Z} \exp(-\mathbf{Z} \cdot \mathbf{Z} - i\mathbf{\tilde{V}} \cdot \mathbf{Z}) \mathcal{Y}_{LM}(\mathbf{Z}_1).
\]

(61)
with \( \alpha = (\tilde{u}A^{-1}u)^{-1/2} \) and \( V = UD^{-1/2}T\pi \).

Since the integral is separable for each variable, the rest of the proof is quite easy. \( N - 1 \) integrals, corresponding to \( Z_k, k > 1 \) are equal to

\[
(2\pi)^{-3/2} \int dZ_k \exp(-Z_k^2 - iV_k \cdot Z_k) = 2^{-3/2} \exp(-V_k^2/4)
\]

while the integral relative to \( Z_1 \) can be calculated using expression (65) to get

\[
(2\pi)^{-3/2} \int dZ_1 \exp(-Z_1^2 - iV_1 \cdot Z_1) \psi_{LM}(Z_1) = (-i)^L 2^{-L-3/2} \exp(-V_1^2/4) \psi_{LM}(V_1).
\]

(63)

Grouping all the exponentials into a single one gives an exponential with the argument \(-\sum V_i^2/4 = -(\mathbf{V} \cdot \mathbf{V})/4 = -(\tilde{\mathbf{\pi}} \cdot \mathbf{A}^{-1}\mathbf{\pi})/4 \). Thus, the final result for the FT looks like

\[
h_{0LM}(u, A; \pi) = (-i)^L e^{-\frac{\tilde{\mathbf{\pi}} \cdot \mathbf{A}^{-1}\mathbf{\pi}}{2L+3N/2}} \psi_{LM}(\tilde{u}A^{-1}\pi).
\]

(64)

It is remarkable that, in this special case \( K = 0 \), the FT of a correlated gaussian is proportional to a correlated gaussian since we have the property

\[
h_{0LM}(u, A; \pi) = (-i)^L \frac{2L+3N/2}{\det A}^{3/2} f_{0LM}(A^{-1}u, A^{-1}A^{-1/4}A).
\]

(65)

With this relationship, it is instructive to check the conservation of the norm, namely \( N_L = \langle f_{0LM} | f_{0LM} \rangle = \langle h_{0LM} | h_{0LM} \rangle \).

We are interested now in the expression of the FT for the most general correlated gaussian

\[
h_{KLM}(u, A; \pi) = \langle \pi | \psi_{KLM}(u, A) \rangle = \int e^{-i\tilde{\mathbf{\pi}} \cdot \mathbf{x}} \psi_{KLM}(u, A; \mathbf{x}) d\mathbf{x}.
\]

(66)

\[
(2\pi)^{-3N/2} \int e^{-i\tilde{\mathbf{\pi}} \cdot \mathbf{x}} f_{KLM}(u, A; \mathbf{x}) d\mathbf{x}.
\]

The principle for the proof is quite similar to what was proposed previously; the same changes of variables occur; the only difference concerns the integration over the \( Z_1 \) variable that must be done now with help of the most general formula (58).

The FT for the general correlated gaussian takes the form

\[
h_{KLM}(u, A; \pi) = \frac{(-i)^L K! (\tilde{u}A^{-1}u)^K}{2L+3N/2 \det A}^{3/2} \psi_{LM}(\tilde{u}A^{-1}\pi).
\]

(67)

\[
\times L^{L+1/2} \left( \frac{\tilde{u}A^{-1}\pi}{4\tilde{u}A^{-1}u} \right)^{2L} e^{-\frac{\tilde{\mathbf{\pi}} \cdot \mathbf{A}^{-1}\mathbf{\pi}}{2L+3N/2}} \psi_{LM}(\tilde{u}A^{-1}\pi).
\]

In this case, the FT of a general correlated gaussian is not proportional to a general correlated gaussian.

However, using the series expansion for the Laguerre polynomial

\[
L_n^m(z) = \sum_{m=0}^{n} (-1)^m \frac{\Gamma(n + a + 1)}{\Gamma(m + a + 1)} \frac{z^m}{m!}.
\]

(68)

it follows that the FT of a general correlated gaussian is a linear combination of general correlated gaussians. Explicitly we have the property

\[
h_{KLM}(u, A; \pi) = \frac{(-i)^L}{(2L+3N/2 \det A)^{3/2}} \sum_{K'=0}^{K} \frac{(-1)^{K'} K!}{K!(K-K')!} \times \frac{(2K + 2L + 1)!}{(2K' + 2L + 1)!} \frac{(\tilde{u}A^{-1}u)^{K-K'} K!}{2^{K+K'+L}} f_{K'LM}(A^{-1}u, A^{-1}A^{-1/4}A).
\]

(69)

VIII. RELATIVISTIC KINETIC ENERGY

In many cases, the potential, or any operator, depends on the momenta \( \pi_i = -i\partial/\partial x_i \). If this dependence occurs through an integer power of the momenta, the method explained above, for example in section IV, applies. However this is not always the case. For such a delicate situation, there is only one remedy : to work in momentum representation.

Let us suppose that the operator \( \hat{O} \) depends on an argument of type \( \tilde{\omega} \pi \). Then the calculation of the matrix element \( \langle \psi_{KLM} | \hat{O} | \psi_{KLM} \rangle = \langle \tilde{h}_{KLM}(u', A'; \pi) | \hat{O} | \psi_{KLM}(u, A; \pi) \rangle \) can be performed using the expansion (69). The dynamical element to be calculated has a form like

\[
(\tilde{f}_{K'LM}(A^{-1}u', A'^{-1}A'^{-1/4}A, \pi) | \hat{O} | \tilde{f}_{KLM}(A^{-1}u, A^{-1}A^{-1/4}A, \pi))\]

(70)

This last element is then computed by application of Eq. (47) (or Eq. (39)) with the trivial changes \( u \rightarrow A^{-1}u \), \( A \rightarrow A^{-1}A'^{-1}A' \rightarrow A'^{-1}A' \rightarrow A'^{-1} \).

As an example of application, we consider the relativistic kinetic energy operator

\[
T_R = \sum_{i=1}^{N+1} \sqrt{p_i^2 + m_i^2}.
\]

(71)

The separation of the center of mass motion cannot be done properly in this case. The usual way to consider the intrinsic motion for the system is to work in the center of mass frame (which is well defined even in the special case where all particles have a vanishing mass); this means that we put \( \mathbf{P} = 0 \) in the subsequent formulae. In particular the momentum \( p_i \) relative to the particle \( i \) writes (see relation (7))

\[
p_i = \sum_{j=1}^{N} U_j^{(i)} \pi_j = U^{(i)} \pi
\]

(72)
with
\[
U^{(i)}_j = \begin{cases} 0 & \text{if } j < i - 1, \\ -1 & \text{if } j = i - 1, \\ \frac{m_i}{m_{12-j}} & \text{if } j \geq i. 
\end{cases}
\] (73)

In order to present simple formulae, let us focus on the special case \( K = K' = 0 \). Then
\[
\langle \psi_{0LM} (u', A') | T_R | \psi_{0LM} (u, A) \rangle = \sum_{i=1}^{N+1} \left( \frac{N_i}{\sqrt{4\pi}} \right) \sum_{k=0}^{L} \frac{2^k (2n+1)!(L-n)!}{Z_i^{3/2}} \times \mathcal{F} \left( 2n+2, \frac{1}{4Z_i}, m_i \right) \left( \frac{\gamma_i' \gamma_i}{\rho} \right)^n \left( 1 - \frac{2Z_i \gamma_i' \gamma_i}{\rho} \right)^{L-n} \frac{U^{(i)} A'B^{-1} u'}{Z_i}. \] (75)

The computation of the matrix element in the summation is performed first using Eq. (65) and then Eq. (45) with the appropriate parameters.

The final result looks like
\[
\langle \psi_{0LM} (u', A') | T_R | \psi_{0LM} (u, A) \rangle = \sum_{i=1}^{N+1} \left( \frac{N_i}{\sqrt{4\pi}} \right) \sum_{k=0}^{L} \frac{2^k (2n+1)!(L-n)!}{Z_i^{3/2}} \times \mathcal{F} \left( 2n+2, \frac{1}{4Z_i}, m_i \right) \left( \frac{\gamma_i' \gamma_i}{\rho} \right)^n \left( 1 - \frac{2Z_i \gamma_i' \gamma_i}{\rho} \right)^{L-n} \frac{U^{(i)} A'B^{-1} u'}{Z_i}. \] (75)

The result can be simplified by using the modified Bessel function. The integral for higher \( l \) can be obtained by the following recursion formula
\[
I_l = \frac{1}{A} I_{l-1} + \frac{(2l-1)(l+1-2\beta)}{A^2} I_{l-2}. \] (79)

All the above formulae allows to get a very efficient way to calculate the matrix element of the relativistic energy operator for the few-body problem expressed in terms of correlated gaussians.

**IX. CONCLUDING REMARKS**

In this paper, we propose a number of new formulae concerning correlated gaussians that cannot be found in SV. Our formulation deals with general correlated gaussians (arbitrary number of particles, arbitrary orbital angular momentum, arbitrary value of the quantum number \( K \)), but is limited to the natural parity states and to operators that do not mix spin and space degrees of freedom.

We present new formulae relative to central potentials. Instead of integrals containing Hermite polynomials, we proposed new formulae with simpler integrals which, most of the time, can be evaluated analytically. Moreover, we derived another formulation for the matrix elements which is more efficient than that presented in SV. All these formulae can be simplified a lot in the special case \( K = K' = 0 \).

But the most interesting point of this paper is the derivation of the Fourier transform of correlated gaussians. In the peculiar case \( K = 0 \), we showed that the Fourier transform is just proportional to a correlated gaussian, but with renormalized parameters. In the general case, we showed that the Fourier transform is a combination of general correlated gaussians.

These new formulae allow the evaluation of the matrix elements of a relativistic kinetic energy operator. Since this kind of operator is more and more introduced in realistic situations, the results of this paper are of primordial importance for future few-body calculations.

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