Analytic matrix elements with shifted correlated Gaussians

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Abstract
Matrix elements between shifted correlated Gaussians of various potentials with several form-factors are calculated analytically. Analytic matrix elements are of importance for the correlated Gaussian method in quantum few-body physics.

1 Introduction
Correlated Gaussian method is a popular variational method to solve quantum-mechanical few-body problems in molecular, atomic, and nuclear physics [1, 2]. One of the important advantages of the correlated Gaussian method is the ease of computing the matrix elements. In some cases the matrix elements and even their gradients with respect to optimization parameters are fully analytic [2, 3, 4, 5]. This enables extensive numerical optimizations to be carried out leading to accurate results [6, 7, 8] despite the incorrect functional form of the Gaussians in certain asymptotic regions of the configuration space.

Although a number of analytic matrix elements have been calculated for different potentials and different forms of correlated Gaussians, one combination — short-range potentials with shifted correlated Gaussians — is still missing [1]. Indeed historically the shifted Gaussians have been applied more often to Coulombic systems rather than to atomic and nuclear systems where the short-range interactions are most important.

In this paper several types of short-range potentials are considered in a search for the form-factors that produce analytic matrix elements with shifted correlated Gaussians. A brief introduction to the correlated Gaussian method is given first and then the analytic matrix elements are introduced.

2 Correlated Gaussian method
Correlated Gaussian method is a variational method where the coordinate part of the wave-function of a quantum few-body system is expanded in terms of correlated Gaussians. Various forms of correlated Gaussians have been conceived [1], one of them being the shifted correlated Gaussian, $|g\rangle$, which for a system of $N$ particles with coordinates $\vec{r}_i, i=1...N$ has the form

$$
\langle r | g \rangle = \exp \left( - \sum_{i,j=1}^{N} A_{ij} \vec{r}_i \cdot \vec{r}_j + \sum_{i=1}^{N} s_i \cdot \vec{r}_i \right) \equiv e^{-r^T A r + s^T r},
$$

(1)

where $r$ is size-$N$ column of particle coordinates $\vec{r}_i$, $A = \{A_{ij}\}$ is a size-$N$ square symmetric positive-definite correlation matrix, $s$ is size-$N$ column of shift vectors $s_i$, and where the following notation has been introduced,

$$
r^T A r \equiv \sum_{i,j=1}^{N} A_{ij} \vec{r}_i \cdot \vec{r}_j, \quad s^T r \equiv \sum_{i=1}^{N} s_i \cdot \vec{r}_i,
$$

(2)

where "." denotes the dot-product of two vectors. The elements of the correlation matrix and the shift vectors are the non-linear parameters of the Gaussians.
The coordinate part of the few-body wave-function $|\psi\rangle$ is represented as a linear combination of several Gaussians,

$$|\psi\rangle = \sum_{i=1}^{n_g} c_i |g_i\rangle,$$

where the coefficients $c_i$ are the linear parameters, and where $n_g$ is the number of Gaussians. Inserting this representation into the Schrödinger equation,

$$\hat{H} |\psi\rangle = E |\psi\rangle,$$

where $\hat{H}$ is the Hamiltonian of the few-body system, and multiplying from the left with $\langle g_j |$ leads to the generalized matrix eigenvalue equation,

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

where $c = \{c_i\}$ is the column of the linear parameters, and where the Hamilton matrix $\mathcal{H} = \{\mathcal{H}_{ij}\}$ and the overlap matrix $\mathcal{N} = \{\mathcal{N}_{ij}\}$ are given as

$$\mathcal{H}_{ij} = \langle g_i | \hat{H} | g_j \rangle, \quad \mathcal{N}_{ij} = \langle g_i | g_j \rangle.$$

The linear parameters together with the energy spectrum are found by solving the generalized eigenvalue problem \[5\] numerically using the standard linear algebra methods \[9\]. The non-linear parameters are optimized by one of many optimization methods which typically involve elements of stochastic-evolutionary \[10\] and direct optimization algorithms \[7\] \[8\]. The direct optimization algorithms often employ gradients of the matrix elements with respect to the optimization parameters.

These optimization techniques involve numerous evaluations of the Hamiltonian matrix elements and their gradients. Therefore the analytically matrix elements are of particular importance for the method.

3 Matrix elements

3.1 Overlap

The overlap $\langle g' | g \rangle$ between a shifted Gaussian $|g\rangle$ with parameters $A$, $s$ and a shifted Gaussian $|g'\rangle$ with parameters $A'$, $s'$ is given as\(^1\)

$$\langle g' | g \rangle = e^{\frac{1}{2}v^T B^{-1} v} \left( \frac{\pi^N}{\det(B)} \right)^{3/2} M,$$

where $B = A' + A$, $v = s' + s$.

3.2 Kinetic energy

The non-relativistic kinetic energy operator $\hat{K}$ for an $N$-body system of particles with coordinates $\vec{r}_i$ and masses $m_i$ is given as

$$\hat{K} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial \vec{r}_i^2}.$$

For completeness we shall consider a more general form of the kinetic energy operator,

$$\hat{K} = -\sum_{i,j=1}^{N} \frac{\partial}{\partial \vec{r}_i} \Lambda_{ij} \frac{\partial}{\partial \vec{r}_j} \equiv -\frac{\partial}{\partial \vec{r}} \Lambda \frac{\partial}{\partial \vec{r}},$$

\(^1\) The overlap can be evaluated by an orthogonal coordinate transformation, $r = Qx$, to the basis where the matrix $B$ is diagonal: $B = QDQ^T$ where $Q^T Q = QQ^T = 1$ and $D$ is a diagonal matrix,

$$\langle g' | g \rangle = \int d^3 \vec{r}_1 \ldots d^3 \vec{r}_N \exp\left(-\vec{r}^T B \vec{r} + v^T r\right) = \int d^3 \vec{x}_1 \ldots d^3 \vec{x}_N \exp\left(-\sum_{i=1}^{N} \vec{x}_i \cdot D_{ii} \vec{x}_i + \sum_{i=1}^{N} \vec{v}_i \cdot \vec{x}_i\right)$$

$$= \prod_{i=1}^{N} \int d^3 \vec{x}_i \exp\left(-\vec{x}_i \cdot D_{ii} \vec{x}_i + \vec{v}_i \cdot \vec{x}_i\right) \left(\frac{\pi}{D_{ii}}\right)^{3/2} = e^{\frac{1}{2}v^T B^{-1} v} \left(\frac{\pi^N}{\det(B)}\right)^{3/2}.$$
efficiently using the update formulas,  

\[ \left\langle g' \left| -\frac{\partial}{\partial r^T} \Lambda \frac{\partial}{\partial r} \right| g \right\rangle = \left\langle g' \left| (s^T - 2r^T A') \Lambda(s - 2A r) \right| g \right\rangle \]

\[ = (6 \text{trace}(A' \Lambda A B^{-1}) + (s' - 2A'u)^T \Lambda(s - 2Au)) M, \tag{14} \]

where \( u = \frac{1}{2} B^{-1} v \), and \( M \) is the overlap.

### 3.3 Potential energy

#### 3.3.1 Central potential

A one-body central potential, \( V(\vec{r}) \), and a two-body central potential, \( V(\vec{r}_i - \vec{r}_j) \), can be written in a convenient general form, \( V(w^T r) \), where \( w \) is a size-\( N \) column of numbers with all components equal zero except for \( w_i = 1 \) for the one-body potential and \( w_i = -w_j = 1 \) for the two-body potential.

**Gaussian form-factor** For the Gaussian form-factor, \( V(w^T r) \propto e^{-\gamma w^T w^T r} \), the matrix element directly follows from the overlap integral,

\[ \left\langle g' \left| e^{-\gamma w^T w^T r} \right| g \right\rangle = e^{\frac{1}{2}B^{-1}v} \left( \frac{\pi^N}{\det(B)} \right)^{3/2} \equiv M', \tag{15} \]

where the matrix \( B' \) is a rank-1 update of the matrix \( B = A' + A, B' = B + \gamma ww^T \).

If the determinant and the inverse of the matrix \( B \) are known, their rank-1 updates can be calculated efficiently using the update formulas,

\[ \det(B + ab^T) = (1 + b^T B^{-1} a) \det(B), \tag{16} \]

\[ (B + ab^T)^{-1} = B^{-1} - \frac{B^{-1}ab^T B^{-1}}{1 + b^T B^{-1} a}, \tag{17} \]

where \( a \) and \( b \) are size-\( N \) columns of numbers.

**Oscillator form-factor** Another potential with a simple analytic matrix element is the oscillator potential, \( V(w^T r) \propto r^T ww^T r \), relevant for cold atoms in traps. The matrix element directly follows from (12),

\[ \left\langle g' \left| r^T ww^T r \right| g \right\rangle = \left( \frac{3}{2} w^T B^{-1} w + u^T ww^T u \right) M. \tag{18} \]

\(^2 \text{We first calculate two integrals,}\)

\[ \left\langle g' \left| r \right| g \right\rangle = \left( \frac{\partial}{\partial v} \right) e^{\frac{1}{2}B^{-1}v} \left( \frac{\pi^N}{\det(B)} \right)^{3/2} = \left( \frac{\partial}{\partial v} \right) e^{\frac{1}{2}B^{-1}v} \left( \frac{\pi^N}{\det(B)} \right)^{3/2}, \tag{11} \]

where \( u = \frac{1}{2} B^{-1} v \), and

\[ \left\langle g' \left| r^T F r \right| g \right\rangle = \left( \frac{\partial}{\partial v} F \frac{\partial}{\partial v^T} \right) e^{\frac{1}{2}B^{-1}v} \left( \frac{\pi^N}{\det(B)} \right)^{3/2} = \left( \frac{3}{2} \text{trace}(FB^{-1}) + u^T F u \right) e^{\frac{1}{2}B^{-1}v} \left( \frac{\pi^N}{\det(B)} \right)^{3/2}, \tag{12} \]

from which the sought integral,

\[ \left\langle g' \left| -\frac{\partial}{\partial r^T} \Lambda \frac{\partial}{\partial r} \right| g \right\rangle = \left\langle g' \left| (s' - 2A'e) \Lambda(s - 2Ar) \right| g \right\rangle, \tag{13} \]

follows directly.
Other analytic form-factors  For a potential with a general form-factor, \( V \propto f(w^T r) \), the matrix element reduces to a three-dimensional integral\(^3\)

\[
\langle g' | f(w^T r) | g \rangle = M \left( \frac{\beta}{\pi} \right)^2 \int d^3 r f(r) e^{-\beta (r - \vec{q})^2},
\]

where \( \beta = (w^T B^{-1} w)^{-1} \) and \( \vec{q} = w^T u \).

If the potential does not depend on the direction of its argument the integral reduces further to a one-dimensional integral,

\[
\langle g' | f(|w^T r|) | g \rangle = M \left( \frac{\beta}{\pi} \right)^2 \frac{2 \pi}{\beta q} \int_0^\infty r dr f(r) e^{-\beta r^2 \sinh(2 \beta q r)}
\]

\( \equiv M J[f] \),

where

\[
J[f] = \left( \frac{\beta}{\pi} \right)^2 \frac{2 \pi}{\beta q} \int_0^\infty r dr f(r) e^{-\beta r^2 \sinh(2 \beta q r)}.
\]

The integral \(^2\) gives relatively simple analytic results for the Coulomb form-factor, \(1/r\),

\[
J \left[ \frac{1}{r} \right] = \frac{\text{erf}(\sqrt{\beta} q)}{q} \rightarrow \frac{2}{\sqrt{\pi}} \sqrt{\beta},
\]

and for several short-range form-factors:

- screened Yukawa, \( e^{-\gamma r^2 - \mu r}/r \),

\[
J \left[ \frac{e^{-\gamma r^2 - \mu r}}{r} \right] = \frac{\sqrt{\beta} e^{-\frac{\beta q^2}{2q}}}{2q \sqrt{\beta + \gamma}} \left( e^{\frac{(\mu - 2 \beta q)^2}{2(\beta + \gamma)}} \left( \text{erf} \left( \frac{2 \beta q - \mu}{2 \sqrt{\beta + \gamma}} \right) + 1 \right) + e^{\frac{(\mu + 2 \beta q)^2}{2(\beta + \gamma)}} \left( \text{erf} \left( \frac{\mu + 2 \beta q}{2 \sqrt{\beta + \gamma}} \right) - 1 \right) \right),
\]

- Yukawa, \( e^{-\mu r}/r \),

\[
J \left[ \frac{e^{-\mu r}}{r} \right] = \lim_{\gamma \to 0} J \left[ \frac{e^{-\gamma r^2 - \mu r}}{r} \right] = \frac{e^{\frac{\mu^2}{2q}}}{2q} \left( 1 - e^{2\mu q} + \text{erf} \left( \frac{2 \beta q - \mu}{2 \sqrt{\beta}} \right) + e^{2\mu q} \text{erf} \left( \frac{2 \beta q + \mu}{2 \sqrt{\beta}} \right) \right),
\]

- screened Coulomb, \( e^{-\gamma r^2}/r \),

\[
J \left[ \frac{e^{-\gamma r^2}}{r} \right] = \lim_{\mu \to 0} J \left[ \frac{e^{-\gamma r^2 - \mu r}}{r} \right] = \sqrt{\beta} e^{-\frac{\beta q^2}{2 \sqrt{\beta + \gamma}}} \frac{\text{erf} \left( \frac{\beta q}{\sqrt{\beta + \gamma}} \right)}{q \sqrt{\beta + \gamma}},
\]

\( ^3 \) Suppose the form-factor \( f(\vec{r}) \) has a Fourier-transform \( \mathcal{F}(\vec{k}) \), then

\[
\langle g' | f(w^T r) | g \rangle = \int d^3 k \mathcal{F}(\vec{k}) \langle g' | e^{i \vec{k} \cdot \vec{r}} | g \rangle = \frac{e^{(w^T B^{-1} w)^{1/2}}}{\det(B)} \int \frac{d^3 \vec{q}}{(2\pi)^3} \mathcal{F}(\vec{k}) e^{-\alpha \vec{k}^2 + i \vec{q} \cdot \vec{k}}
\]

where \( \alpha = \frac{1}{4} w^T B^{-1} w, \vec{q} = \frac{1}{2} w^T B^{-1} \vec{v} \). Now the last integral can as well be written as

\[
\left( \frac{\beta}{\pi} \right)^2 \int d^3 r f(r) e^{-\beta (r - \vec{q})^2},
\]

where \( \beta = \frac{1}{4\alpha} = (w^T B^{-1} w)^{-1} \).
3.3.2 Tensor potential

The tensor potential \( V_1 \) between two particles with coordinates \( \vec{r}_1, \vec{r}_2 \) and spins \( \vec{S}_1, \vec{S}_2 \) can be written in the form

\[
V_1(r) \propto f(r)(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}),
\]

where \( \vec{r} = \vec{r}_1 - \vec{r}_2 \) is the relative coordinate between the particles, and \( f(r) \) is the radial form-factor of the potential. In this form the potential has a central spin-spin component,

\[
\frac{1}{3} f(r) r^2 (\vec{S}_1 \cdot \vec{S}_2),
\]

which is often subtracted from the above form to make sure the potential contains only the spherical tensor component.

Introducing the size-\( N \) column of numbers \( w \),

\[
w = \{w_i|w_1 = 1, w_2 = -1, w_{i\neq1,2} = 0\},
\]

and vector-columns \( y_1 = \vec{S}_1 w, \ y_2 = \vec{S}_2 w \), the tensor potential can be written in a convenient general form,

\[
\hat{V}_1 \propto f(w^T r)(y_1^T r)(y_2^T r),
\]

where

\[
y_i^T r = \sum_{i=1}^N \vec{y}_i \cdot \vec{r}_i.
\]
The tensor matrix element can be represented as a derivative of the central matrix element with the same form-factor,

\[
\langle g' \mid f(w^T r)(y_1^T r)(y_2^T r) \mid g \rangle = \left( y_1^T \frac{\partial}{\partial v_1} \right) \left( y_2^T \frac{\partial}{\partial v_2} \right) \langle g' \mid f(w^T r) \mid g \rangle .
\]  

(38)

The central part (36) of the tensor potential has a similar analytic representation,

\[
\langle g' \mid f(w^T r)(w^T r) \mid g \rangle = \left( w^T \frac{\partial}{\partial v_1} \right) \left( w^T \frac{\partial}{\partial v_1} \right) \langle g' \mid f(w^T r) \mid g \rangle .
\]  

(39)

Thus if the matrix element of the central potential with a given form-factor \( f \) is analytic, the matrix element of the tensor potential \( f(w^T r)(y_1^T r)(y_2^T r) \) is also analytic. In particular, the tensor matrix elements of the screened Yukawa form-factor and its descendants (32) are also analytic.

**Gaussian form-factor** For a Gaussian form-factor the matrix elements (38,39) are readily given as

\[
\langle g' \mid e^{-\beta w^T w} \cdot (y_1^T r)(y_2^T r) \mid g \rangle = \left( \frac{1}{2} y_1^T B'^{-1} y_2 + (y_1^T u')(y_2^T u') \right) M',
\]

\[
\langle g' \mid e^{-\beta w^T w} \cdot (r^T w^T r) \mid g \rangle = \left( \frac{3}{2} w^T B'^{-1} w + u'^T w u' \right) M',
\]

where \( B' = B + \gamma w^T, B = A' + A, u' = \frac{1}{2} B'^{-1} v, v = s + s, \) and where

\[
M' = e^{\frac{\beta}{3} \langle v^T B'^{-1} v \rangle} \left( \frac{\pi^N}{\det(B')} \right)^{3/2}
\]

(40)

is the central Gaussian matrix element.

Again the updates \( \det(B + \gamma w w^T) \) and \( (B + \gamma w w^T)^{-1} \) can be efficiently calculated using rank-1 update formulas.

**Other form-factors** The tensor matrix element (38) can be written in component form as

\[
\langle g' \mid f(w^T r)(y_1^T r)(y_2^T r) \mid g \rangle = \sum_{i,j=1}^{N} \sum_{a,b=1}^{3} \langle \tilde{r}_i \rangle_{i,a} \langle \tilde{y}_2 \rangle_{j,b} \langle g' \mid f(w^T r) \tilde{r}_a \tilde{r}_b \mid g \rangle
\]

\[
= \sum_{i,j=1}^{N} \sum_{a,b=1}^{3} \langle \tilde{y}_i \rangle_{i,a} \langle \tilde{y}_2 \rangle_{j,b} \frac{\partial}{\partial v_{i,a}} \frac{\partial}{\partial v_{j,b}} \langle g' \mid f(w^T r) \mid g \rangle .
\]

(41)

where \( \tilde{r}_a \) is the number-\( a \) component of the vector \( \tilde{r} \), and where

\[
\langle g' \mid f(w^T r) \mid g \rangle = M J,
\]

\[
M = e^{\frac{\beta}{3} \langle v^T B^{-1} v \rangle} \left( \frac{\pi^N}{\det(B)} \right)^{\frac{1}{2}}
\]

(43)

\[
J = \left( \frac{\beta}{\pi} \right)^{\frac{3}{2}} 2\pi e^{-\frac{\beta}{2q}} \int_0^{\infty} r dr f(r) e^{-\beta r^2} \sinh(2\beta qr).
\]

(44)

The derivative of the central matrix element at the right-hand side of (41) can now be evaluated as

\[
\left( \frac{\partial}{\partial v_{i,a}} \frac{\partial}{\partial v_{j,b}} M \right) J + M \left( \frac{\partial}{\partial v_{i,a}} \frac{\partial}{\partial v_{j,b}} \frac{\partial}{\partial v_{i,a}} \frac{\partial}{\partial v_{j,b}} J \right)
\]

\[
+ \left( \frac{\partial}{\partial v_{i,a}} M \right) \left( \frac{\partial}{\partial v_{j,b}} J \right)
\]

(45)

6
\[
\frac{\partial}{\partial \vec{v}_{ia}} M = \sum_{k=1}^{N} \frac{1}{2} B^{-1}_{ik} \vec{v}_{ka} M,
\]
(46)
\[
\frac{\partial}{\partial \vec{v}_{ja}} \frac{\partial}{\partial \vec{v}_{ia}} M = \frac{1}{2} B^{-1}_{ji} \delta_{ab} + \sum_{k,l=1}^{N} \frac{1}{2} B^{-1}_{ik} \vec{v}_{ka} \frac{1}{2} B^{-1}_{jl} \vec{v}_{lb} M,
\]
(47)
\[
\frac{\partial}{\partial \vec{v}_{ia}} J = \frac{\partial J}{\partial \vec{v}_{ia}},
\]
(48)
\[
\frac{\partial}{\partial \vec{v}_{ia}} \frac{\partial}{\partial \vec{v}_{ja}} J = \frac{\partial^2 J}{\partial q^2} \frac{\partial q_j}{\partial \vec{v}_{ja}} \frac{\partial q_i}{\partial \vec{v}_{ia}} + \frac{\partial J}{\partial \vec{v}_{ja}} \frac{\partial^2 q_j}{\partial \vec{v}_{ja} \partial \vec{v}_{ia}},
\]
(49)
\[
\frac{\partial q_j}{\partial \vec{v}_{ia}} = \frac{1}{q} \sum_{k=1}^{N} h_k \vec{v}_{ka},
\]
(50)
\[
\frac{\partial^2 q_j}{\partial \vec{v}_{ja} \partial \vec{v}_{ia}} = \frac{1}{q} h_i h_j \delta_{ab} - \frac{2}{q^2} \sum_{k=1}^{N} h_k \vec{v}_{ka} \sum_{l=1}^{N} h_j h_l \vec{v}_{lb}.
\]
(51)

where \(h = w^T B^{-1} \).

Now to finish the calculation one only needs to calculate \(\partial J/\partial q\) and \(\partial^2 J/\partial q^2\) for the given potential. For the screened Yukawa form-factor and its descendants \(\delta^2 J/\partial q^2\) are analytic although the actual calculations are relatively tedious and should be best performed by a computer algebra software like Maxima \([12]\). For example, the expression for

\[
\frac{\partial^2 J}{\partial q^2} \left[ \frac{e^{-\gamma r^2 - \mu r}}{r} \right]
\]
(52)

can be readily obtained by the following Maxima script,

\[
\text{assume(beta>0, gamma>0, mu>0, q>0);}
\]
\[
\text{J(f) := (beta/pi)^3/2*2*pi/beta/q*exp(-beta*q^2)*integrate(r*f*exp(-beta*r^2)*sinh(2*beta*q*r),r,0,inf);} \]
\[
\text{fortran(diff(J(exp(-gamma*r^2-mu*r)/r), q, 2))};
\]

which analytically calculates \(\delta^2 J/\partial q^2\) for the screened Yukawa potential and outputs the corresponding Fortran code.

Even if \(J\) is not analytic one can evaluate its derivatives by calculating numerically a few extra integrals,

\[
\frac{\partial J}{\partial q} = -2 \sqrt{\beta} e^{-\beta q^2} \int_0^\infty r e^{-\beta r^2} f(r) \sinh(2\beta qr) \, dr
\]
\[
= 4 \beta^2 e^{-\beta q^2} \int_0^\infty r e^{-\beta r^2} f(r) \sinh(2\beta qr) \, dr
\]
\[
= 4 \beta^2 e^{-\beta q^2} \int_0^\infty r^2 e^{-\beta r^2} f(r) \cosh(2\beta qr) \, dr
\]
(53)
\[
\frac{\partial^2 J}{\partial q^2} = \frac{8 \beta^2 e^{-\beta q^2}}{\sqrt{\pi} q} \int_0^\infty \frac{r^3 e^{-\beta r^2} f(r) \sinh (2 \beta qr) \, dr}{\sqrt{\pi} q} + \frac{4 \beta^2 e^{-\beta q^2}}{\sqrt{\pi} q} \int_0^\infty \frac{r^3 e^{-\beta r^2} f(r) \sinh (2 \beta qr) \, dr}{\sqrt{\pi} q} \]
\[
+ \frac{4 \sqrt{3} e^{-\beta q^2}}{\sqrt{\pi} q^3} \int_0^\infty r^2 e^{-\beta r^2} f(r) \cosh (2 \beta qr) \, dr - \frac{8 \beta^2 e^{-\beta q^2}}{\sqrt{\pi} q^2} \int_0^\infty r^2 e^{-\beta r^2} f(r) \cosh (2 \beta qr) \, dr - \frac{16 \beta^2 e^{-\beta q^2}}{\sqrt{\pi} q^2} \int_0^\infty r^2 e^{-\beta r^2} f(r) \cosh (2 \beta qr) \, dr.
\]

(54)

3.3.3 Spin-orbit potential

The spin-orbit potential between two particles with coordinates \( \vec{r}_1 \) and \( \vec{r}_2 \) and spins \( \vec{S}_1 \) and \( \vec{S}_2 \) can be written in the form

\[
V_{so} \propto f(r) \left( \vec{S} \cdot \vec{L} \right),
\]

(55)

where \( \vec{r} = \vec{r}_1 - \vec{r}_2 \) is the relative coordinate between the particles; \( f(r) \) is the radial form-factor of the potential; \( \vec{S} = \vec{S}_1 + \vec{S}_2 \) is the total spin of the two particles; and \( \vec{L} \) is the relative orbital momentum between the two particles,

\[
\vec{L} = (\vec{r}_1 - \vec{r}_2) \times -\frac{i}{2} \left( \frac{\partial}{\partial \vec{r}_1} - \frac{\partial}{\partial \vec{r}_2} \right),
\]

(56)

where “\( \times \)” denotes vector-product of two vectors.

The orbital momentum operator can be written, using the size-\( N \) column of numbers \( w \),

\[
w = \{ w_i \, | w_1 = 1, w_2 = -1, w_{i \neq 1,2} = 0 \},
\]

(57)

in the general form,

\[
\vec{L} = -\frac{i}{2} \left( w^T \vec{r} \times \vec{r} \frac{\partial}{\partial \vec{r}^T} \right),
\]

(58)

where

\[
w^T \vec{r} \equiv \sum_{i=1}^N w_i \vec{r}_i, \quad w^T \frac{\partial}{\partial \vec{r}} \equiv \sum_{i=1}^N w_i \frac{\partial}{\partial \vec{r}_i}.
\]

(59)

For a given form-factor \( f(w^T \vec{r}) \) the spin-orbit matrix element can be represented through the central matrix element with the same form-factor,

\[
\left\langle g' \mid f(w^T \vec{r}) \left( w^T \vec{r} \times \vec{r} \frac{\partial}{\partial \vec{r}^T} \right) \mid g \right\rangle = \left( w^T \frac{\partial}{\partial \vec{r}^T} \right) \times w^T \left( s - 2A \frac{\partial}{\partial \vec{r}^T} \right) \left( g' \mid f(w^T \vec{r}) \mid g \right),
\]

(60)

so that if the central matrix element is analytic — as is the case for the screened Yukawa form-factor and its descendants — the spin-orbit matrix element is also analytic.

**Gaussian form-factor** For a Gaussian form-factor the spin-orbit matrix element is given as

\[
\left\langle g' \mid e^{-\gamma w^T \vec{r}} \left( w^T \vec{r} \times \vec{r} \frac{\partial}{\partial \vec{r}^T} \right) \mid g \right\rangle = \frac{1}{2} w^T B'^{-1} v \times (w^T s - w^T A B'^{-1} v) M',
\]

(61)

where \( B' = B + \gamma w^T \), \( B' = A' + A \), \( u' = \frac{1}{2} B'^{-1} v \), \( v = s' + s \), and where
\[ M' = e^{\frac{1}{4} \gamma B'^{-1}} \left( \frac{\pi^N}{\det(B')} \right)^{3/2} \]

is the central Gaussian matrix element.

Again \( \det(B') \) and \( B'^{-1} \) can be efficiently calculated using rank-1 update formulas.

**General form-factor** The component number \( a \) of the spin-orbit matrix element \([60]\) can be written in component form as

\[
\langle g' | f(w^T r) \left( w^T r \times w^T \frac{\partial}{\partial r} \right)_a | g \rangle = \sum_{b,c=1}^{3} \epsilon_{abc} \sum_{k=1}^{N} w_k \frac{\partial}{\partial v_k b} \sum_{l=1}^{N} w_l \left( s_{lc} - 2 \sum_{j=1}^{N} A_{lj} \frac{\partial}{\partial v_j c} \right) \langle g' | f(w^T r) | g \rangle .
\]

(64)

It is clearly a linear combination of the first, \( \frac{\partial}{\partial v_k b} \langle g' | f(w^T r) | g \rangle \), and second, \( \frac{\partial}{\partial v_j c} \frac{\partial}{\partial v_k b} \langle g' | f(w^T r) | g \rangle \), derivatives of the corresponding central matrix element \( \langle g' | f(w^T r) | g \rangle = MJ \). These quantities have been calculated in the previous chapter.

### 3.4 Many-body forces

Many-body potentials in nuclear physics have form-factors which depend on the coordinates of several nucleons. In addition they may have tensor and spin-orbit post-factors.

For a many-body potential with a Gaussian form-factor, \( e^{-r^T W r} \), where \( W \) is a symmetric positive-definite matrix, the central matrix element is given as

\[
\langle g' | e^{-r^T W r} | g \rangle = e^{\frac{1}{4} \gamma (B + W)^{-1}} \left( \frac{\pi^N}{\det(B + W)} \right)^{3/2} .
\]

(65)

The simple tensor and spin-orbit post-factors can be calculated in the same way as has been done in the previous two chapters.

### 4 Conclusion

In quantum few-body physics the analytic matrix elements are of importance for the correlated Gaussians method as they facilitate extensive numerical optimizations of the variational wave-functions. In this paper it has been shown that potentials in the form

\[
f(w^T r), f(w^T r)(y^T r)(z^T r), f(w^T r)(a^T r)(b^T r), f(w^T r) \left( w^T r \times w^T \frac{\partial}{\partial r} \right) ,
\]

(66)

have analytic matrix elements between shifted correlated Gaussians for the following class of form-factors,

\[
f(r) = r^n e^{-\gamma r^2 - \mu r} f\left( \frac{\partial}{\partial r} \right), \ n = 0, 1, \ldots
\]

(67)

Of these form-factors the Gaussian form-factors produce particularly simple and concise analytic expressions. Therefore an efficient strategy could be to represent the potentials at hand as linear combinations of Gaussians and then use the analytic expressions for the Gaussians.

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