



Timothy Zaklama · David Zhang · Keefer Rowan ·
Louis Schatzki · Yasuyuki Suzuki · Kálmán Varga 

Matrix Elements of One Dimensional Explicitly Correlated Gaussian Basis Functions

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Abstract Kinetic, potential and overlap matrix elements of one dimensional correlated Gaussians multiplied by polynomial factors are presented. These matrix elements can be used to calculate energies of one dimensional cold atom systems, or to construct a tensorial product to calculate energies in 2 or 3 dimensional systems with a nonspherical potential.

1 Introduction

The experimental realization of one-dimensional (1D) cold atomic systems [1–7] has sparked an intense theoretical interest in 1D few particle systems [8–14]. High accuracy calculations of energies and wave functions of few-body systems have been continuously developed [15–32] for three dimensional system and many of these approaches can be used in 1D as well.

Two- and three-electron atomic systems can be very accurately calculated using Hylleraas-type functions [33,34], but the extension of the Hylleraas basis approach beyond three electrons is very tedious due to the difficulty of the analytical calculation of their matrix elements [35]. Explicitly Correlated Gaussian (ECG) basis functions have no such restrictions, and have become very popular tools in high accuracy calculations [36–49,49,50,50–56]. There are several recent reviews illustrating the wide range of applications of ECGs [30,57,58].

ECGs as basis functions were first employed in 1960 by Boys [15] and Singer [16]. The simple quadratic form involving inter-particle distances in ECGs permits the reduction of the matrix elements to simple analytic expressions, and the algebraic complexity does not change with the number of particles. These matrix elements depend on the parameters of the ECGs, which should be carefully optimized [41,59,60] to get highly accurate variational upper bounds.

In this paper we present detailed derivations of matrix elements of one-dimensional generalized ECGs: ECGs multiplied with a polynomial prefactor formed by the powers of the coordinates of the particles. The polynomial prefactor not only helps the accuracy, but allows for the treatment of spin-orbit interaction or calculation of matrix elements of the dipole operator of a laser field. While the matrix elements presented in this work are in 1D, they can be simply generalized to 2D or 3D by using their tensor products. These tensor products can be used in calculations of systems in nonspherical potentials (e.g. electric or magnetic fields) and can also be used to derive general 3D ECG basis functions with arbitrary angular momentum after suitable angular momentum coupling. In our earlier work [61], we have derived matrix elements of ECGs in 3D for

K. Varga (✉) · T. Zaklama · D. Zhang · K. Rowan · L. Schatzki
Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, USA
E-mail: kalman.varga@vanderbilt.edu

Y. Suzuki
Department of Physics, Niigata University, Niigata, Japan

arbitrary angular momentum; the present work extends this to nonspherical potentials and gives a general form for 1D systems.

The outline of the paper is as follows: After the introduction we will introduce our notation and formalism, and will give calculations for different operators, such as overlap, kinetic energy, one-particle and two-particle potentials in later sections.

2 Formalism

We consider a system of N particles in 1D space, with positions in a lab-frame Cartesian coordinate system given by x_i , $i = 1, \dots, N$. To simplify the notation we introduce

$$\mathbf{x} = (x_1, \dots, x_N). \quad (1)$$

The ECG basis functions are defined as

$$\Phi_{\mathbf{m}}^A(\mathbf{x}) = \left[\prod_{k=1}^N x_k^{m_k} \right] \exp \left(-\frac{1}{2} \mathbf{x}^T A \mathbf{x} \right), \quad (2)$$

where the quadratic form in the exponent is defined as

$$\mathbf{x}^T A \mathbf{x} := \sum_{i,j=1}^N A_{ij} x_i \cdot x_j. \quad (3)$$

Recall that $\mathbf{x} \in \mathbb{R}^N$ is a vector in the configuration space of N particles, each moving in one dimension, $A \in \mathbb{R}^{N \times N}$ is a matrix of variational parameters, and $\mathbf{m} \in \mathbb{Z}_{\geq 0}^N$ is a vector of polynomial exponents. To ensure that these functions are normalizable, we require that A be positive-definite. Without loss of generality we can take A to be symmetric.

We will consider a Hamiltonian in the lab frame defined as

$$\begin{aligned} H &= T + U_{\text{One-Body}} + V_{\text{Two-Body}} \\ &= \sum_{i=1}^N \frac{p_i^2}{2m_i} + \sum_{i=1}^N U(x_i) + \sum_{i<j}^N V(x_i - x_j), \end{aligned}$$

where $p_k = -i\hbar d/dx_k$ is the momentum operator for the i th particle.

3 Overlap Matrix Elements

In this section we compute the matrix elements of the one-dimensional ECG basis functions.

To evaluate these matrix elements, we introduce the *generating function*

$$G_{\mathbf{t}}^A(\mathbf{x}) = \exp \left(-\frac{1}{2} \mathbf{x}^T A \mathbf{x} + \mathbf{t}^T \mathbf{x} \right) \quad (4)$$

where $\mathbf{t} \in \mathbb{R}^N$ is a vector of parameters. Observe that the basis functions $\Phi_{\mathbf{m}}^A(\mathbf{x})$ can be expressed as derivatives of $G_{\mathbf{t}}^A(\mathbf{x})$:

$$\Phi_{\mathbf{m}}^A(\mathbf{x}) = \left[\prod_{k=1}^N \frac{\partial^{m_k}}{\partial t_k^{m_k}} \right] G_{\mathbf{t}}^A(\mathbf{x}) \Big|_{\mathbf{t}=\mathbf{0}} \quad (5)$$

Thus, our strategy will be to first evaluate the matrix elements $\langle G_{\mathbf{t}}^A \hat{O} G_{\mathbf{t}'}^{A'} \rangle$ of the generating functions, and then take derivatives with respect to the parameters t_k to obtain the matrix elements $\langle \Phi_{\mathbf{m}}^A \hat{O} \Phi_{\mathbf{m}'}^{A'} \rangle$ of the ECG basis functions.

We first calculate the overlap matrix element. The overlap of two generating functions is simply a multi-dimensional Gaussian integral:

$$\langle G_{\mathbf{t}}^A | G_{\mathbf{t}'}^{A'} \rangle = \sqrt{\frac{(2\pi)^N}{\det B}} \exp\left(\frac{1}{2}(\mathbf{t} + \mathbf{t}')^T B^{-1}(\mathbf{t} + \mathbf{t}')\right) \quad (6)$$

Here we have defined $B = A + A'$. (Note that the invertibility of B is guaranteed by A and A' being positive-definite.) This can be written in a more concise form by introducing the $2N$ -dimensional vector

$$\underline{\mathbf{t}} = \begin{bmatrix} \mathbf{t} \\ \mathbf{t}' \end{bmatrix} = [t_1 \cdots t_N \ t'_1 \cdots t'_N]^T \quad (7)$$

and the $2N \times 2N$ block matrix

$$\underline{B} = \begin{bmatrix} B^{-1} & B^{-1} \\ B^{-1} & B^{-1} \end{bmatrix}. \quad (8)$$

(Henceforth we will use underlined symbols to denote $2N$ -dimensional vectors or matrices obtained in this fashion, by concatenating the N variables in the bra and the N variables in the ket.) By using these notations, we have

$$\begin{aligned} \langle G_{\mathbf{t}}^A | G_{\mathbf{t}'}^{A'} \rangle &= \sqrt{\frac{(2\pi)^N}{\det B}} \exp\left(\frac{1}{2} \underline{\mathbf{t}}^T \underline{B} \underline{\mathbf{t}}\right) \\ &= \sqrt{\frac{(2\pi)^N}{\det B}} \exp\left(\frac{1}{2} \sum_{i,j=1}^{2N} \underline{B}_{ij} t_i t_j\right). \end{aligned} \quad (9)$$

The overlap of the basis functions then can be calculated from

$$\begin{aligned} \langle \Phi_{\mathbf{m}}^A | \Phi_{\mathbf{m}'}^{A'} \rangle &= \left[\prod_{k=1}^N \frac{\partial^{m_k}}{\partial t_k^{m_k}} \right] \left[\prod_{k=1}^N \frac{\partial^{m'_k}}{\partial t'_k^{m'_k}} \right] \langle G_{\mathbf{t}}^A | G_{\mathbf{t}'}^{A'} \rangle \Big|_{\mathbf{t}=\mathbf{t}'=\mathbf{0}} \\ &= \left[\prod_{k=1}^{2N} \frac{\partial^{m_k}}{\partial t_k^{m_k}} \right] \langle G_{\mathbf{t}}^A | G_{\mathbf{t}'}^{A'} \rangle \Big|_{\underline{\mathbf{t}}=\mathbf{0}}. \end{aligned} \quad (10)$$

To evaluate these derivatives, we begin by Taylor-expanding the exponential function in equation (9). This allows us to write

$$\langle G_{\mathbf{t}}^A | G_{\mathbf{t}'}^{A'} \rangle = \sqrt{\frac{(2\pi)^N}{\det B}} \prod_{i,j=1}^{2N} \sum_{k_{ij}=0}^{\infty} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} t_i t_j \right)^{k_{ij}} \quad (11)$$

Now, we expand out the product $\prod_{i,j=1}^{2N}$ and push all the summation operators to the front, obtaining

$$\langle G_{\mathbf{t}}^A | G_{\mathbf{t}'}^{A'} \rangle = \sqrt{\frac{(2\pi)^N}{\det B}} \sum_{k_{11}=0}^{\infty} \sum_{k_{12}=0}^{\infty} \cdots \sum_{k_{2N,2N}=0}^{\infty} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} t_i t_j \right)^{k_{ij}}. \quad (12)$$

In the preceding equation there are a total of $(2N)^2$ summation operators, one for each variable k_{ij} , $i, j = 1, \dots, 2N$. Equivalently, if we let $\mathbb{Z}_{\geq 0}^{2N \times 2N}$ denote the set of $2N \times 2N$ matrices with nonnegative integer entries, we can write this as

$$\langle G_{\mathbf{t}}^A | G_{\mathbf{t}'}^{A'} \rangle = \sqrt{\frac{(2\pi)^N}{\det B}} \sum_{k \in \mathbb{Z}_{\geq 0}^{2N \times 2N}} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} t_i t_j \right)^{k_{ij}}. \quad (13)$$

Thus we have:

$$\begin{aligned} \langle \Phi_{\mathbf{m}}^A | \Phi_{\mathbf{m}'}^{A'} \rangle &= \left[\prod_{k=1}^{2N} \frac{\partial^{m_k}}{\partial t_k^{m_k}} \right] \langle G_{\mathbf{t}}^A | G_{\mathbf{t}'}^{A'} \rangle \Big|_{\mathbf{t}=\mathbf{0}} = \sqrt{\frac{(2\pi)^N}{\det B}} \sum_{k \in \mathbb{Z}_{\geq 0}^{2N \times 2N}} \\ &\quad \left[\prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} B_{ij} \right)^{k_{ij}} \right] \left[\prod_{p=1}^{2N} \frac{\partial^{m_p}}{\partial t_p^{m_p}} \right] \left[\prod_{i,j=1}^{2N} (t_i t_j)^{k_{ij}} \right] \Big|_{\mathbf{t}=\mathbf{0}}. \end{aligned} \quad (14)$$

This can be evaluated by observing that

$$\prod_{i,j=1}^{2N} (t_i t_j)^{k_{ij}} = \prod_{p=1}^{2N} t_p^{\sum_{q=1}^{2N} (k_{qp} + k_{pq})} = \prod_{p=1}^{2N} t_p^{u_p} \quad (15)$$

where we have defined the abbreviation $u_p = \sum_{q=1}^{2N} (k_{qp} + k_{pq})$. It follows that

$$\begin{aligned} \left[\prod_{k=1}^{2N} \frac{\partial^{m_k}}{\partial t_k^{m_k}} \right] \left[\prod_{i,j=1}^{2N} (t_i t_j)^{k_{ij}} \right] &= \prod_{p=1}^{2N} \frac{\partial^{m_p}}{\partial t_p^{m_p}} t_p^{u_p} \\ &= \prod_{p=1}^{2N} u_p (u_p - 1) \cdots (u_p - m_p + 1) t_p^{u_p - m_p}. \end{aligned} \quad (16)$$

Now consider what happens when we set $\mathbf{t} = \mathbf{0}$. The expression (16) is nonzero only when $u_p = m_p$ for all $p = 1, \dots, 2N$, since in this case $t_p^{u_p - m_p} = 0^0 = 1$. This means that the infinite sum (14) reduces to a finite sum, since the only terms that contribute are those in which the numbers $\{k_{ij}\}_{i,j=1}^{2N}$ are arranged in such a way that

$$\sum_{q=1}^{2N} (k_{qp} + k_{pq}) = m_p \quad \text{for all } p = 1, \dots, 2N. \quad (17)$$

This leads us naturally to the following combinatorial problem:

Definition Given a vector $\mathbf{m} \in \mathbb{Z}_{\geq 0}^n$ of n nonnegative integers, let $\Omega(\mathbf{m})$ be the set of $n \times n$ matrices $k \in \mathbb{Z}_{\geq 0}^{n \times n}$ having nonnegative integer entries such that $\sum_{q=1}^{2N} (k_{qp} + k_{pq}) = m_p$ for all $p = 1, \dots, 2N$.

We will return to this combinatorial problem later in ‘‘Appendix A’’. For now, let us assume that we know how to compute $\Omega(\underline{\mathbf{m}})$, and use this to simplify the infinite sum (13). We obtain the formula

$$\begin{aligned} \langle \Phi_{\mathbf{m}}^A | \Phi_{\mathbf{m}'}^{A'} \rangle &= \left[\prod_{k=1}^{2N} \frac{\partial^{m_k}}{\partial t_k^{m_k}} \right] \langle G_{\mathbf{t}}^A | G_{\mathbf{t}'}^{A'} \rangle \Big|_{\mathbf{t}=\mathbf{0}} \\ &= \sqrt{\frac{(2\pi)^N}{\det B}} \left(\prod_{p=1}^{2N} m_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} B_{ij} \right)^{k_{ij}} \end{aligned} \quad (18)$$

completing the derivation of the overlap matrix element.

4 Kinetic Energy Matrix Elements

The kinetic energy matrix elements can be evaluated using the generating function:

$$\langle G_t^A | T | G_{t'}^{A'} \rangle = - \sum_{i=1}^N \frac{\hbar^2}{2m} \langle G_t^A | \frac{\partial^2}{\partial x_i^2} | G_{t'}^{A'} \rangle. \quad (19)$$

This can be calculated in two equivalent ways, either taking the second derivative on one side or taking first derivative on both sides.

The first, direct evaluation, gives:

$$\frac{\partial^2 G_t^A}{\partial x_i^2} = (t_i^2 + (Ax)_i^2 - 2t_i(Ax)_i - A_{ii})G_t^A, \quad (20)$$

and

$$\langle G_t^A | T | G_{t'}^{A'} \rangle = -\frac{\hbar^2}{2m} \langle G_t^A | t'^T t' + x^T A'^2 x - 2t'^T A' x - \text{Tr}(A') | G_{t'}^{A'} \rangle \quad (21)$$

This can be calculated using the integral given in “Appendix B”, and the final result is:

$$-\frac{\hbar^2}{2m} \langle G_t^A | G_{t'}^{A'} \rangle (t'^T t' - \text{Tr}(A') - 2t'^T A' B^{-1}(\mathbf{t} + \mathbf{t}') + \text{Tr}(A'^2 B^{-1}) + (\mathbf{t} + \mathbf{t}')^T B^{-1} A'^2 B^{-1}(\mathbf{t} + \mathbf{t}')). \quad (22)$$

Using the second approach, by integration by parts (neglecting the boundary term as $G \rightarrow 0$ as $\mathbf{x} \rightarrow \infty$), we have

$$\langle G_t^A | \frac{\partial^2}{\partial x_i^2} | G_{t'}^{A'} \rangle = - \left\langle \frac{\partial G_t^A}{\partial x_i} \left| \frac{\partial G_{t'}^{A'}}{\partial x_i} \right. \right\rangle. \quad (23)$$

Using

$$\frac{\partial G_t^A}{\partial x_i} = (\mathbf{t} - A\mathbf{x})_i G_t^A. \quad (24)$$

we have

$$\begin{aligned} \langle G_t^A | T | G_{t'}^{A'} \rangle &= \frac{\hbar^2}{2m} \langle G_t^A | (\mathbf{t} - A\mathbf{x}) \cdot (\mathbf{t}' - A'\mathbf{x}) | G_{t'}^{A'} \rangle \\ &= \frac{\hbar^2}{2m} \langle G_t^A | \mathbf{t} \cdot \mathbf{t}' + \mathbf{x}^T A A' \mathbf{x} - (\mathbf{t}^T A' + \mathbf{t}'^T A) \mathbf{x} | G_{t'}^{A'} \rangle. \end{aligned} \quad (25)$$

For the the quadratic term we can use the integral presented in “Appendix B”, for the linear terms we note

$$\begin{aligned} \int_{\mathbb{R}^n} x_i \exp\left(-\frac{1}{2}\mathbf{x}^T A \mathbf{x} + \mathbf{s}^T \mathbf{x}\right) d\mathbf{x} &= \frac{\partial}{\partial s_i} \int_{\mathbb{R}^n} \exp\left(-\frac{1}{2}\mathbf{x}^T A \mathbf{x} + \mathbf{s}^T \mathbf{x}\right) d\mathbf{x} \\ &= \frac{\partial}{\partial s_i} \sqrt{\frac{(2\pi)^n}{\det A}} \exp\left(\frac{1}{2}\mathbf{s}^T A^{-1} \mathbf{s}\right) \\ &= \sqrt{\frac{(2\pi)^n}{\det A}} \exp\left(\frac{1}{2}\mathbf{s}^T A^{-1} \mathbf{s}\right) (A^{-1} \mathbf{s})_i. \end{aligned} \quad (26)$$

Then, similarly to above, Eq. (25) evaluates to:

$$\begin{aligned} \frac{\hbar^2}{2m} \langle G_t^A | G_{t'}^{A'} \rangle [&\mathbf{t} \cdot \mathbf{t}' \\ &+ \text{Tr}(A A' B^{-1}) + (\mathbf{t} + \mathbf{t}')^T B^{-1} A A' B^{-1}(\mathbf{t} + \mathbf{t}') \\ &- (\mathbf{t}^T A' + \mathbf{t}'^T A) B^{-1}(\mathbf{t} + \mathbf{t}')]. \end{aligned} \quad (27)$$

Both Eqs. (27) and (22) are valid derivations for the kinetic energy for the generator functions. We have included both because they can be useful in calculations, for example for checking computer codes.

Now, to find the matrix elements of the basis, we apply derivatives to the matrix elements of the generating function:

$$\langle \Phi_m^A | T | \Phi_{m'}^{A'} \rangle = \prod_{k=1}^{2N} \frac{\partial^{m_k}}{\partial t_k^{m_k}} \langle G_t^A | T | G_{t'}^{A'} \rangle \Big|_{t=0, t'=0}, \quad (28)$$

We will use the expression in (27) to find the kinetic matrix elements because it gives a manifestly symmetric result. Expanding Eq. (27) in terms of sums and derivatives:

$$\begin{aligned}
& \frac{\hbar^2}{2m} \langle G_t^A | G_t^{A'} \rangle \left(\sum_{i=1}^N (AA'B^{-1})_{ii} + \sum_{i=1}^N t_i t'_i - \sum_{i,j=1}^{2N} C_{ij} t_i t_j + \sum_{i,j=1}^{2N} D_{ij} t_i t_j \right) \\
&= \frac{\hbar^2}{2m} \sqrt{\frac{(2\pi)^N}{\det B}} \left(\sum_{i=1}^N (AA'B^{-1})_{ii} + \sum_{j=1}^N \frac{\partial}{\partial \underline{B}_{j,j+N}} \right. \\
&\quad \left. - \sum_{i,j=1}^{2N} C_{ij} \frac{\partial}{\partial \underline{B}_{ij}} + \sum_{i,j=1}^{2N} D_{ij} \frac{\partial}{\partial \underline{B}_{ij}} \right) \exp \left\{ \frac{1}{2} \sum_{i,j=1}^{2N} \underline{B}_{ij} t_i t_j \right\} \quad (29)
\end{aligned}$$

Where

$$C = \begin{pmatrix} A'B^{-1} & A'B^{-1} \\ AB^{-1} & AB^{-1} \end{pmatrix}, \quad D = \begin{pmatrix} B^{-1}AA'B^{-1} & B^{-1}AA'B^{-1} \\ B^{-1}AA'B^{-1} & B^{-1}AA'B^{-1} \end{pmatrix} \quad (30)$$

Pulling the sum out of the exponent and Taylor expanding, (29) takes on the form:

$$\begin{aligned}
&= \frac{\hbar^2}{2m} \sqrt{\frac{(2\pi)^N}{\det B}} \left(\sum_{i=1}^N (AA'B^{-1})_{ii} + \sum_{j=1}^N \frac{\partial}{\partial \underline{B}_{j,j+N}} \right. \\
&\quad \left. - \sum_{i,j=1}^{2N} C_{ij} \frac{\partial}{\partial \underline{B}_{ij}} + \sum_{i,j=1}^{2N} D_{ij} \frac{\partial}{\partial \underline{B}_{ij}} \right) \prod_{i,j=1}^{2N} \sum_{k_{ij}=0}^{\infty} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} t_i t_j \right)^{k_{ij}}. \quad (31)
\end{aligned}$$

Expanding the product and pushing all the summations to the front,

$$\begin{aligned}
&= \frac{\hbar^2}{2m} \sqrt{\frac{(2\pi)^N}{\det B}} \left(\sum_{i=1}^N (AA'B^{-1})_{ii} + \sum_{j=1}^N \frac{\partial}{\partial \underline{B}_{j,j+N}} \right. \\
&\quad \left. - \sum_{i,j=1}^{2N} C_{ij} \frac{\partial}{\partial \underline{B}_{ij}} + \sum_{i,j=1}^{2N} D_{ij} \frac{\partial}{\partial \underline{B}_{ij}} \right) \sum_{k_{11}=0}^{\infty} \sum_{k_{12}=0}^{\infty} \cdots \sum_{k_{2N,2N}=0}^{\infty} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} t_i t_j \right)^{k_{ij}}. \quad (32)
\end{aligned}$$

This can be written, using the shorthand notation from the overlap evaluation as

$$\begin{aligned}
&= \frac{\hbar^2}{2m} \sqrt{\frac{(2\pi)^N}{\det B}} \left(\sum_{i=1}^N (AA'B^{-1})_{ii} + \sum_{j=1}^N \frac{\partial}{\partial \underline{B}_{j,j+N}} \right. \\
&\quad \left. - \sum_{i,j=1}^{2N} C_{ij} \frac{\partial}{\partial \underline{B}_{ij}} + \sum_{i,j=1}^{2N} D_{ij} \frac{\partial}{\partial \underline{B}_{ij}} \right) \sum_{k \in \mathbb{Z}_{\geq 0}^{2N \times 2N}} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} t_i t_j \right)^{k_{ij}}. \quad (33)
\end{aligned}$$

To find the matrix elements of the basis, we apply derivatives to matrix elements of the generating function

$$\begin{aligned}
& \left[\prod_{k=1}^{2N} \frac{\partial m_k}{\partial t_k} \right] \frac{\hbar^2}{2m} \sqrt{\frac{(2\pi)^N}{\det B}} \left(\sum_{i=1}^N (AA'B^{-1})_{ii} + \sum_{j=1}^N \frac{\partial}{\partial \underline{B}_{j,j+N}} \right. \\
& \quad \left. - \sum_{i,j=1}^{2N} C_{ij} \frac{\partial}{\partial \underline{B}_{ij}} + \sum_{i,j=1}^{2N} D_{ij} \frac{\partial}{\partial \underline{B}_{ij}} \right) \sum_{k \in \mathbb{Z}_{\geq 0}^{2N \times 2N}} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} t_i t_j \right)^{k_{ij}} \\
& = \frac{\hbar^2}{2m} \sqrt{\frac{(2\pi)^N}{\det B}} \left(\sum_{i=1}^N (AA'B^{-1})_{ii} + \sum_{j=1}^N \frac{\partial}{\partial \underline{B}_{j,j+N}} \right. \\
& \quad \left. - \sum_{i,j=1}^{2N} C_{ij} \frac{\partial}{\partial \underline{B}_{ij}} + \sum_{i,j=1}^{2N} D_{ij} \frac{\partial}{\partial \underline{B}_{ij}} \right) \sum_{k \in \mathbb{Z}_{\geq 0}^{2N \times 2N}} \prod_{i,j=1}^{2N} \left[\frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} \right)^{k_{ij}} \right] \left[\prod_{k=1}^{2N} \frac{\partial m_k}{\partial t_k} \right] \prod_{i,j=1}^{2N} (t_i t_j)^{k_{ij}},
\end{aligned} \tag{34}$$

which, similar to the overlap case, becomes:

$$\begin{aligned}
& = \frac{\hbar^2}{2m} \sqrt{\frac{(2\pi)^N}{\det B}} \left(\sum_{i=1}^N (AA'B^{-1})_{ii} + \sum_{j=1}^N \frac{\partial}{\partial \underline{B}_{j,j+N}} \right. \\
& \quad \left. - \sum_{i,j=1}^{2N} C_{ij} \frac{\partial}{\partial \underline{B}_{ij}} + \sum_{i,j=1}^{2N} D_{ij} \frac{\partial}{\partial \underline{B}_{ij}} \right) \left(\prod_{p=1}^{2N} \underline{m}_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} \right)^{k_{ij}}.
\end{aligned} \tag{35}$$

After distributing the terms, we have

$$\begin{aligned}
& = \frac{\hbar^2}{2m} \sqrt{\frac{(2\pi)^N}{\det B}} \left(\sum_{i=1}^N \text{Tr}(AA'B^{-1}) \left[\left(\prod_{p=1}^{2N} \underline{m}_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} \right)^{k_{ij}} \right] \right. \\
& \quad + \sum_{j=1}^N \frac{\partial}{\partial \underline{B}_{j,j+N}} \left[\left(\prod_{p=1}^{2N} \underline{m}_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} \right)^{k_{ij}} \right] \\
& \quad - \sum_{i,j=1}^{2N} C_{ij} \frac{\partial}{\partial \underline{B}_{ij}} \left[\left(\prod_{p=1}^{2N} \underline{m}_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} \right)^{k_{ij}} \right] \\
& \quad \left. + \sum_{i,j=1}^{2N} D_{ij} \frac{\partial}{\partial \underline{B}_{ij}} \left[\left(\prod_{p=1}^{2N} \underline{m}_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} \right)^{k_{ij}} \right] \right)
\end{aligned} \tag{36}$$

Finally, differentiating, we arrive at our final result:

$$\begin{aligned}
\langle \Phi_m^A | T | \Phi_m^{A'} \rangle & = \frac{\hbar^2}{2m} \sqrt{\frac{(2\pi)^N}{\det B}} \left(\text{Tr}(AA'B^{-1}) \left(\prod_{p=1}^{2N} \underline{m}_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} \right)^{k_{ij}} \right. \\
& \quad + \left(\prod_{p=1}^{2N} \underline{m}_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \frac{\prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} \underline{B}_{ij} \right)^{k_{ij}}}{\prod_{j=1}^N \frac{1}{k_{j,j+N}!} \left(\frac{1}{2} \underline{B}_{j,j+N} \right)^{k_{j,j+N}}} \left(\prod_{j=1}^N \frac{1}{(k_{j,j+N} - 1)!} \left(\frac{1}{2} \right)^{k_{j,j+N}} (\underline{B}_{j,j+N})^{k_{j,j+N}-1} \right) \\
& \quad \left. + \left(\sum_{i,j=1}^{2N} D_{ij} - \sum_{i,j=1}^{2N} C_{ij} \right) \left(\prod_{p=1}^{2N} \underline{m}_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \prod_{i,j=1}^{2N} \frac{1}{(k_{ij} - 1)!} \left(\frac{1}{2} \right)^{k_{ij}} (\underline{B}_{ij})^{k_{ij}-1} \right)
\end{aligned} \tag{37}$$

5 Potential Energy Matrix Elements

To calculate the matrix elements of the one-body U and two-body potential V we will use the following expressions

$$\sum_{k=1}^N U(x_k) = \sum_{k=1}^N \int U(x) \delta(x_k - x) dx = \sum_{k=1}^N \int U(x) \delta(w^{(k)}_x - x) dx \quad (38)$$

where

$$w^{(k)}_x = \sum_{i=1}^N w_i^{(k)} x_i \quad w_i^{(k)} = \delta_{ki} \quad (39)$$

and

$$\sum_{k < l}^N V(x_{kl}) = \sum_{k < l}^N \int V(x) \delta(x_k - x_l - x) dx = \sum_{k < l}^N \int V(x) \delta(w^{(kl)}_x - x) dx \quad (40)$$

where

$$w^{(kl)}_x = \sum_{i=1}^N w_i^{(kl)} x_i \quad w_i^{(kl)} = \delta_{ki} - \delta_{li}. \quad (41)$$

These equations show that by calculating the matrix elements of

$$\delta(wx - x) \quad (42)$$

one can evaluate both the one-body and two-body integrals. The matrix element of $\delta(wx - x)$:

$$\langle G_t^A | \delta(wx - x) | G_{t'}^{A'} \rangle = \sqrt{\frac{c}{2\pi}} \exp \left\{ -\frac{c}{2} (x - wB^{-1}(t + t'))^2 \right\} \langle G_t^A | G_{t'}^{A'} \rangle \quad (43)$$

where

$$c = \frac{1}{w^T B^{-1} w}. \quad (44)$$

This matrix element can be written as

$$\begin{aligned} \langle G_t^A | \delta(wx - x) | G_{t'}^{A'} \rangle &= \sqrt{\frac{c}{2\pi}} \exp \left\{ -\frac{c}{2} x^2 \right\} \sqrt{\frac{(2\pi)^N}{\det B}} \times \\ &\exp \left\{ \frac{1}{2} \sum_{i,j=1}^{2N} \underline{B}'_{ij} t_i t_j + \sum_{j=1}^{2N} x c e_j t_j \right\}, \end{aligned} \quad (45)$$

where

$$e = \underline{B}w, \underline{w} = \begin{bmatrix} w \\ w \end{bmatrix} = [w_1 \cdots w_N \ w_1 \cdots w_N]^T \quad (46)$$

and

$$\underline{B}'_{ij} = \underline{B}_{ij} - c e_i e_j. \quad (47)$$

The potential matrix element can be calculated from

$$\langle \Phi_m^A | \delta(wx - x) | \Phi_{m'}^{A'} \rangle = \prod_{k=1}^{2N} \frac{\partial^{m_k}}{\partial t_k^{m_k}} \langle G_t^A | \delta(wx - x) | G_{t'}^{A'} \rangle \Big|_{t=0, t'=0}, \quad (48)$$

which using the general Leibniz rule, can be written as

$$\begin{aligned}
 \langle \Phi_m^A | \delta(wx - x) | \Phi_{m'}^{A'} \rangle &= \\
 &= \sqrt{\frac{c}{2\pi}} \exp\left\{-\frac{c}{2}x^2\right\} \sqrt{\frac{(2\pi)^N}{\det B}} \prod_{k=1}^{2N} \sum_{n_k=0}^{m_k} \binom{m_k}{n_k} \\
 &\quad \times \frac{\partial^{n_k}}{\partial t_k^{n_k}} \exp\left\{\frac{1}{2} \sum_{i,j=1}^{2N} B'_{ij} t_i t_j\right\} \\
 &\quad \frac{\partial^{m_k-n_k}}{\partial t_k^{m_k-n_k}} \exp\left\{\sum_{j=1}^{2N} x c e_j t_j\right\}. \tag{49}
 \end{aligned}$$

The derivatives of the first exponent are already calculated in Eq. (18). The derivatives of the second exponent can be calculated in a similar way, which eventually produces the following expression

$$\begin{aligned}
 \langle \Phi_m^A | \delta(wx - x) | \Phi_{m'}^{A'} \rangle &= \left[\prod_{k=1}^{2N} \frac{\partial^{m_k}}{\partial t_k^{m_k}} \right] \langle G_t^A | \delta(wx - x) | G_t^{A'} \rangle \Big|_{t=0} \\
 &= \sqrt{\frac{(2\pi)^N}{\det B}} \left(\prod_{p=1}^{2N} m_p! \right) \sum_{k \in \Omega(\underline{\mathbf{m}})} \prod_{i,j=1}^{2N} \frac{1}{k_{ij}!} \left(\frac{1}{2} B'_{ij} \right)^{k_{ij}} \left(\prod_{p=1}^{2N} (m_p - n_p)! \right) \sum_{k \in \Delta(\underline{\mathbf{m}} - \underline{\mathbf{n}})} \prod_{j=1}^{2N} \frac{1}{k_j!} (x c e_j)^{k_j} \tag{50}
 \end{aligned}$$

where $\mathbf{m}, \mathbf{n}$ are vectors $\in \mathbb{Z}_{\geq 0}^n$ of n nonnegative integers. Now let $\Delta(\underline{\mathbf{m}} - \underline{\mathbf{n}})$ be the set of n -dimensional vectors $\mathbf{k} \in \mathbb{Z}_{\geq 0}^n$ having nonnegative integer entries such that $k_p = m_p - n_p$ for all $p = 1, \dots, 2N$, and $\Omega(\underline{\mathbf{m}})$ is defined as it is in the previous section. This completes the derivation of the potential matrix elements.

To calculate the potential matrix elements one has to integrate

$$\int V(x) x^{2n} \exp\left\{-\frac{c}{2}x^2\right\} dx. \tag{51}$$

This can easily be calculated analytically or numerically for many potentials of interest.

6 Numerical Example

To show the usefulness of the matrix elements calculated in this work, we present a simple illustrative example: the calculation of the energy of few electron atoms in 1D. As the Coulomb potential is singular in 1D, we use a soft Coulomb potential

$$U(x_i) = -\frac{Z}{(a^2 + x_i^2)^{1/2}}, \quad V(x_i - x_j) = \frac{1}{(a^1 + (x_i - x_j)^2)^{1/2}} \tag{52}$$

for the one and two-body potentials, respectively ($a = 1$ a.u.).

The wave function of the system is approximated as linear combination of ECGs,

$$\Psi = \sum_i c_i \mathcal{A}\{\Phi_{\mathbf{m}}^{A_i}(\mathbf{x})\}, \tag{53}$$

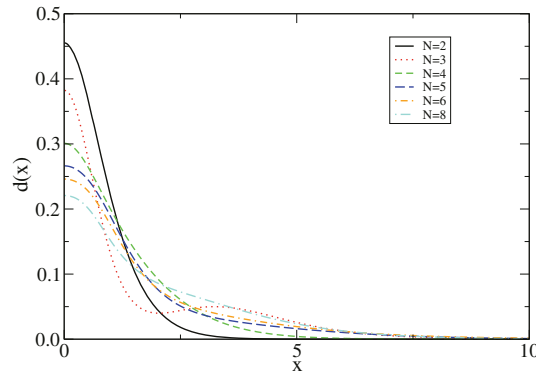
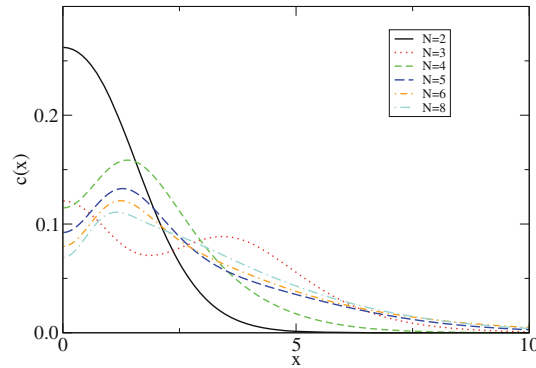
where $\mathcal{A}$ is an antisymmetrizer. The nonlinear parameters, A_i , are optimized with the stochastic variational method [41]. The energy of the 1D atoms are listed in Table 1. These can serve as reference numbers for test calculations in 1D.

We have also calculated the electron density

$$d(x) = \frac{1}{N} \sum_{i=1}^N \langle \Psi | \delta(x_i - x) | \Psi \rangle, \tag{54}$$

Table 1 Ground state energies (in a.u.) of 1D atoms. The spins of the electrons arranged in such a way that $(N-1)/2$ electrons are spin up, the rest is spin down

N	Energy
2	-2.238
3	-4.028
4	-6.785
5	-9.818
6	-13.313
8	-27.378

**Fig. 1** Electron density of 1D atoms (in a.u.)**Fig. 2** Electron correlation of 1D atoms (in a.u.)

and the electron correlation function

$$c(x) = \frac{2}{N(N-1)} \sum_{i < j}^N \langle \Psi | \delta(x_i - x_j - x) | \Psi \rangle. \quad (55)$$

These functions are symmetric with respect to the origin and shown in Figs. 1 and 2.

The densities are very similar for different atoms, except in the $N = 3$ case, where it seems that two electrons remains close to the center and the third electron is pushed outside. The $N > 3$ correlation functions each have their maxima nearly the same distance from the center, which can be easily explained with electron repulsion. The correlation function of the $N = 2$ and $N = 3$ atoms have their maxima at the origin (two electrons with spin up and spin down are distinguishable and can stay close to the center). The $N = 3$ correlation function has a second maximum, around the same position as the $N = 3$ density, showing that the third electron is pushed away from the center.

7 Summary

We have presented the matrix elements of general one dimensional ECGs. These analytical matrix elements can be used in various calculations, for example in 1D cold atom systems. Using these matrix elements, one can also construct matrix elements of 2D or 3D systems by simple tensor products. These matrix elements can be especially useful in calculations where the potential is not spherical, for example in systems in magnetic or electric field. The matrix elements can also be used for spherical system with appropriate angular momentum couplings.

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8 Appendix A

In this appendix we show an example how to generate integers satisfying Eq. (17). First we rewrite Eq. (17) as

$$k_{1,p} + k_{2,p} + \cdots + 2k_{p,p} + \cdots + k_{p,2N} = m_p \quad (56)$$

This equation can be written in form of a linear equation by reindexing $k_{1,p}, \dots, k_{p,2N}$ to form a vector, q , and defining an S matrix for the coefficients of q :

$$\sum_{i=1}^{2N} q_i S_{ip} + \sum_{k=2N+1}^{2N+\frac{2N(2N-1)}{2}} q_k S_{kp} = m_p \quad (57)$$

To illustrate how this can be done we give a $N = 2$ example showing the equivalence between Eqs. (56) and (57).

Starting with Eq. (56) for $N = 2$,

$$\begin{aligned} 2k_{1,1} + k_{1,2} + k_{1,3} + k_{1,4} &= m_1 \\ 2k_{2,2} + k_{1,2} + k_{2,3} + k_{2,4} &= m_2 \\ 2k_{3,3} + k_{1,3} + k_{2,3} + k_{3,4} &= m_3 \\ 2k_{4,4} + k_{1,4} + k_{2,4} + k_{3,4} &= m_4 \end{aligned} \quad (58)$$

Writing out the summations of Eq. (57),

$$\begin{aligned} q_1 S_{1,1} + q_2 S_{2,1} + q_3 S_{3,1} + q_4 S_{4,1} \\ + q_5 S_{5,1} + q_6 S_{6,1} + q_7 S_{7,1} + q_8 S_{8,1} + q_9 S_{9,1} + q_{10} S_{10,1} &= m_1 \end{aligned} \quad (59)$$

$$\begin{aligned} q_1 S_{1,2} + q_2 S_{2,2} + q_3 S_{3,2} + q_4 S_{4,2} \\ + q_5 S_{5,2} + q_6 S_{6,2} + q_7 S_{7,2} + q_8 S_{8,2} + q_9 S_{9,2} + q_{10} S_{10,2} &= m_2 \end{aligned} \quad (60)$$

$$\begin{aligned} q_1 S_{1,3} + q_2 S_{2,3} + q_3 S_{3,3} + q_4 S_{4,3} \\ + q_5 S_{5,3} + q_6 S_{6,3} + q_7 S_{7,3} + q_8 S_{8,3} + q_9 S_{9,3} + q_{10} S_{10,3} &= m_3 \end{aligned} \quad (61)$$

$$\begin{aligned} q_1 S_{1,4} + q_2 S_{2,4} + q_3 S_{3,4} + q_4 S_{4,4} \\ + q_5 S_{5,4} + q_6 S_{6,4} + q_7 S_{7,4} + q_8 S_{8,4} + q_9 S_{9,4} + q_{10} S_{10,4} &= m_4 \end{aligned} \quad (62)$$

To define a mapping between q and k , let $q_i = k_{i,i}$ for $i = 1, 2N$. This is the diagonal of the matrix k . For $i > 2N$, we assign the remaining q_i to the elements for which $i < j$, left to right and top to down (with x denoting redundant elements due to symmetry):

$$\begin{pmatrix} q_1 & q_5 & q_6 & q_7 \\ x & q_2 & q_8 & q_9 \\ x & x & q_3 & q_{10} \\ x & x & x & q_4 \end{pmatrix} \rightarrow \begin{pmatrix} k_{11} & k_{12} & k_{13} & k_{14} \\ x & k_{22} & k_{23} & k_{24} \\ x & x & k_{33} & k_{34} \\ x & x & x & k_{44} \end{pmatrix} \quad (63)$$

Note that q is not a matrix, it is only illustrated this way for clarity.

The selection matrix S contains integer elements of 0, 1, or 2. This will account for (by setting the value of S equal to 0) the extra terms in Eqs. (59)–(62) that are not in Eq. (58), and account for the coefficient of 2 in front of some terms.

Rewriting Eq. (58) with this mapping,

$$\begin{aligned} 2q_1 + q_5 + q_6 + q_7 &= m_1 \\ 2q_2 + q_5 + q_8 + q_9 &= m_2 \\ 2q_3 + q_6 + q_8 + q_{10} &= m_3 \\ 2q_4 + q_7 + q_9 + q_{10} &= m_4 \end{aligned} \quad (64)$$

The matrix S must then be

$$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix} \quad (65)$$

Once the S matrix is defined, Eq. (57) can be solved for any given set of m_p by finding the integers satisfying the equation.

9 Appendix B

In this appendix we show how to calculate a Gaussian integral used in the derivation of the matrix elements. Equations similar to this have been published before (see e.g. in Ref. [41]), but here we prove it for a general complex symmetric matrix.

Let $A \in \mathbb{C}^{N \times N}$ be a complex-symmetric matrix with positive-definite real part. Then for any $Q \in \mathbb{C}^{N \times N}$ and $s \in \mathbb{C}^N$

$$\begin{aligned} & \int_{\mathbb{R}^N} \frac{1}{2} \mathbf{x}^T Q \mathbf{x} \exp \left(-\frac{1}{2} \mathbf{x}^T A \mathbf{x} + \mathbf{s}^T \mathbf{x} \right) d\mathbf{x} \\ &= \sqrt{\frac{2\pi}{\det B}} \exp \left(\frac{1}{2} \mathbf{s}^T A^{-1} \mathbf{s} \right) \left[\frac{1}{2} \text{Tr}(Q A^{-1}) + \frac{1}{2} (A^{-1} \mathbf{s})^T Q (A^{-1} \mathbf{s}) \right] \end{aligned} \quad (66)$$

Proof As in the preceding proof, pick an invertible matrix $V \in \mathbb{R}^{N \times N}$ such that $D \equiv V^T A V$ is diagonal, and let $R \equiv V^T Q V$ and $\mathbf{u} \equiv V^T \mathbf{s}$. Then by performing a change of variable $\mathbf{y} = V^T \mathbf{x}$, we can write

$$\begin{aligned} I &\equiv \int_{\mathbb{R}^N} \frac{1}{2} \mathbf{x}^T Q \mathbf{x} \exp \left(-\frac{1}{2} \mathbf{x}^T A \mathbf{x} + \mathbf{s}^T \mathbf{x} \right) d\mathbf{x} \\ &= \int_{\mathbb{R}^N} \frac{1}{2} \mathbf{x}^T Q \mathbf{x} \exp \left(-\frac{1}{2} \mathbf{x}^T V^{-T} D V^{-1} \mathbf{x} + \mathbf{s}^T \mathbf{x} \right) d\mathbf{x} \\ &= \int_{\mathbb{R}^N} \frac{1}{2} \mathbf{y}^T V^T Q V \mathbf{y} \exp \left(-\frac{1}{2} \mathbf{y}^T D \mathbf{y} + \mathbf{s}^T V \mathbf{y} \right) \det V d\mathbf{y} \\ &= \frac{\det V}{2} \int_{\mathbb{R}^N} \mathbf{y}^T R \mathbf{y} \exp \left(-\frac{1}{2} \mathbf{y}^T R \mathbf{y} + \mathbf{u}^T \mathbf{y} \right) d\mathbf{y} \end{aligned}$$

$$\begin{aligned}
&= \frac{\det V}{2} \int_{\mathbb{R}^N} \sum_{j,k=1}^N R_{jk} y_j y_k \exp \left(\frac{1}{2} \sum_{l=1}^N d_l y_l^2 + \sum_{l=1}^N u_l y_l \right) d\mathbf{y} \\
&= \frac{\det V}{2} \sum_{j,k=1}^N R_{jk} \int_{\mathbb{R}^N} y_j y_k \prod_{l=1}^N \exp \left(-\frac{1}{2} d_l y_l^2 + u_l y_l \right) d\mathbf{y}
\end{aligned} \tag{67}$$

At this point, we consider separately the $j = k$ and $j \neq k$ terms. When $j = k$, we want to evaluate the integral

$$I_j \equiv \int_{\mathbb{R}^N} y_j^2 \prod_{l=1}^N \exp \left(-\frac{1}{2} d_l y_l^2 + u_l y_l \right) d\mathbf{y} \tag{68}$$

Observe that each term with $l \neq j$ contributes a factor of

$$\int_{-\infty}^{\infty} \exp \left(-\frac{1}{2} d_l y_l^2 + u_l y_l \right) dy_l = \sqrt{\frac{2\pi}{d_l}} \exp \left(\frac{u_l^2}{2d_l} \right) \tag{69}$$

while the $l = j$ term contributes a factor of

$$\int_{-\infty}^{\infty} \exp \left(-\frac{1}{2} d_j y_j^2 + u_j y_j \right) dy_j = \left(\frac{d_j + u_j^2}{d_j^2} \right) \sqrt{\frac{2\pi}{d_j}} \exp \left(\frac{u_j^2}{2d_j} \right) \tag{70}$$

multiplying these factors gives the result

$$I_j = \left(\frac{d_j + u_j^2}{d_j^2} \right) \prod_{l=1}^N \sqrt{\frac{2\pi}{d_l}} \exp \left(\frac{u_l^2}{2d_l} \right) = \left(\frac{d_j + u_j^2}{d_j^2} \right) \sqrt{\frac{(2\pi)^N}{\det D}} \exp \left(\frac{1}{2} \mathbf{s}^T A^{-1} \mathbf{s} \right) \tag{71}$$

When $j \neq k$ we want to evaluate the integral

$$I_{jk} \equiv \int_{\mathbb{R}^N} y_j y_k \prod_{l=1}^N \exp \left(-\frac{1}{2} d_l y_l^2 + u_l y_l \right) d\mathbf{y} \tag{72}$$

Again, each term with $l \neq j, k$, contributes a factor of $\sqrt{\frac{2\pi}{d_l}} \exp \left(\frac{u_l^2}{2d_l} \right)$, while the $l = j, k$ terms contribute a factor of

$$\int_{-\infty}^{\infty} y_j \exp \left(-\frac{1}{2} d_j y_j^2 + u_j y_j \right) dy_j = \left(\frac{u_j}{d_j} \right) \sqrt{\frac{2\pi}{d_j}} \exp \left(\frac{u_j^2}{2d_j} \right) \tag{73}$$

Multiplying these factors gives the result

$$I_{jk} = \left(\frac{u_j u_k}{d_j d_k} \right) \prod_{l=1}^N \sqrt{\frac{2\pi}{d_l}} \exp \left(\frac{u_l^2}{2d_l} \right) = \left(\frac{u_j u_k}{d_j d_k} \right) \sqrt{\frac{(2\pi)^N}{\det D}} \exp \left(\frac{1}{2} \mathbf{s}^T A^{-1} \mathbf{s} \right) \tag{74}$$

Returning to the integral, we have

$$\begin{aligned}
 I &= \frac{\det V}{2} \left[\sum_{j=1}^N R_{jj} I_j + \sum_{j \neq k}^N R_{jk} I_{jk} \right] \\
 &= \frac{\det V}{2} \sqrt{\frac{(2\pi)^N}{\det D}} \exp\left(\frac{1}{2} \mathbf{s}^T A^{-1} \mathbf{s}\right) \left[\sum_{j=1}^N R_{jj} \frac{d_j + u_j^2}{d_j^2} + \sum_{j \neq k}^N R_{jk} \frac{u_j u_k}{d_j d_k} \right] \\
 &= \frac{1}{2} \sqrt{\frac{(2\pi)^N}{\det(V^{-T} D V^{-1})}} \exp\left(\frac{1}{2} \mathbf{s}^T A^{-1} \mathbf{s}\right) \left[\sum_{j=1}^N \frac{R_{jj}}{d_j} + \sum_{j,k=1}^N R_{jk} \frac{u_j u_k}{d_j d_k} \right] \\
 &= \sqrt{\frac{(2\pi)^N}{\det D}} \exp\left(\frac{1}{2} \mathbf{s}^T A^{-1} \mathbf{s}\right) \left[\frac{1}{2} \text{Tr}(R D^{-1}) + \frac{1}{2} \mathbf{u}^T D^{-T} T D^{-1} \mathbf{u} \right] \\
 &= \sqrt{\frac{(2\pi)^N}{\det D}} \exp\left(\frac{1}{2} \mathbf{s}^T A^{-1} \mathbf{s}\right) \left[\frac{1}{2} \text{Tr}((V^T Q V)(V^T A V)^{-1}) \right. \\
 &\quad \left. + \frac{1}{2} \mathbf{u}^T (V^T A V)^{-T} (V^T Q V)(V^T A V)^{-1} \mathbf{u} \right] \\
 &= \sqrt{\frac{(2\pi)^N}{\det D}} \exp\left(\frac{1}{2} \mathbf{s}^T A^{-1} \mathbf{s}\right) \left[\frac{1}{2} \text{Tr}(Q A^{-1}) + \frac{1}{2} (A^{-1} \mathbf{s})^T Q (A^{-1} \mathbf{s}) \right], \tag{75}
 \end{aligned}$$

which is the desired result. $\square$

References

1. H. Moritz, T. Stöferle, M. Köhl, T. Esslinger, Phys. Rev. Lett. **91**, 250402 (2003). <https://doi.org/10.1103/PhysRevLett.91.250402>
2. T. Stöferle, H. Moritz, C. Schori, M. Köhl, T. Esslinger, Phys. Rev. Lett. **92**, 130403 (2004). <https://doi.org/10.1103/PhysRevLett.92.130403>
3. T. Kinoshita, T. Wenger, D.S. Weiss, Nature **440**(7086), 900 (2006). <https://doi.org/10.1038/nature04693>
4. T. Kinoshita, T. Wenger, D.S. Weiss, Science **305**(5687), 1125 (2004). <https://doi.org/10.1126/science.1100700>
5. E. Haller, M. Gustavsson, M.J. Mark, J.G. Danzl, R. Hart, G. Pupillo, H.C. Nägerl, Science **325**(5945), 1224 (2009). <https://doi.org/10.1126/science.1175850>
6. G. Pagano, M. Mancini, G. Cappellini, P. Lombardi, F. Schäfer, H. Hu, X.J. Liu, J. Catani, C. Sias, M. Inguscio, L. Fallani, Nature Physics (2014). <https://doi.org/10.1038/nphys2878>
7. B. Paredes, A. Widera, V. Murg, O. Mandel, S. Fölling, I. Cirac, G.V. Shlyapnikov, T.W. Hänsch, I. Bloch, Nature **429**(6989), 277 (2004). <https://doi.org/10.1038/nature02530>
8. D. Pecak, A.S. Dehkarghani, N.T. Zinner, T. Sowinski, Phys. Rev. A **95**, 053632 (2017). <https://doi.org/10.1103/PhysRevA.95.053632>
9. J. Chen, J.M. Schurer, P. Schmelcher, Phys. Rev. A **98**, 023602 (2018). <https://doi.org/10.1103/PhysRevA.98.023602>
10. T. Sowiński, M.Á. García-March, Rep. Prog. Phys. **82**(10), 104401 (2019). <https://doi.org/10.1088/1361-6633/ab3a80>
11. J. von Stecher, C.H. Greene, D. Blume, Phys. Rev. A **77**, 043619 (2008). <https://doi.org/10.1103/PhysRevA.77.043619>
12. D. Rakshit, K.M. Daily, D. Blume, Phys. Rev. A **85**, 033634 (2012). <https://doi.org/10.1103/PhysRevA.85.033634>
13. Y. Ding, C.H. Greene, Phys. Rev. A **95**, 053602 (2017). <https://doi.org/10.1103/PhysRevA.95.053602>
14. Y. Yan, D. Blume, Phys. Rev. A **91**, 043607 (2015). <https://doi.org/10.1103/PhysRevA.91.043607>
15. S.F. Boys, Proc. R. Soc. Lond. Ser. A **258**, 402–411 (1960). <https://doi.org/10.1098/rspa.1960.0195>
16. K. Singer, Proc. R. Soc. Lond. Ser. A **258**, 412–420 (1960). <https://doi.org/10.1098/rspa.1960.0196>
17. W. Kołos, L. Wolniewicz, Rev. Mod. Phys. **35**, 473 (1963). <https://doi.org/10.1103/RevModPhys.35.473>
18. G.W.F. Drake, R.A. Swainson, Phys. Rev. A **44**, 5448 (1991). <https://doi.org/10.1103/PhysRevA.44.5448>
19. Z. Yan, G.W.F. Drake, J. Phys. B **30**, 4723 (1997). <https://doi.org/10.1088/0953-4075/30/21/012>
20. V.I. Korobov, Phys. Rev. A **61**, 064503 (2000)
21. H. Nakatsuji, H. Nakashima, Y. Kurokawa, A. Ishikawa, Phys. Rev. Lett. **99**, 240402 (2007). <https://doi.org/10.1103/PhysRevLett.99.240402>
22. G.G. Ryzhikh, J. Mitroy, Phys. Rev. Lett. **79**, 4124 (1997)
23. S. Bubin, K. Varga, Phys. Rev. A **84**, 012509 (2011). <https://doi.org/10.1103/PhysRevA.84.012509>
24. S. Bubin, L. Adamowicz, J. Chem. Phys. **120**, 6051 (2004)
25. M. Stanke, D. Kędziera, M. Molski, S. Bubin, M. Barysz, L. Adamowicz, Phys. Rev. Lett. **96**, 233002 (2006). <https://doi.org/10.1103/PhysRevLett.96.233002>
26. W. Cencek, J. Komasa, J. Rychlewski, Chem. Phys. Lett. **246**, 417 (1995). [https://doi.org/10.1016/0009-2614\(95\)01146-8](https://doi.org/10.1016/0009-2614(95)01146-8)

27. K.L. Sharkey, N. Kirnosov, L. Adamowicz, J. Chem. Phys. **138**(10), 104107 (2013). <https://doi.org/10.1063/1.4794192>
28. K.L. Sharkey, N. Kirnosov, L. Adamowicz, J. Chem. Phys. **139**(16), 164119 (2013). <https://doi.org/10.1063/1.4826450>
29. N. Kirnosov, K.L. Sharkey, L. Adamowicz, J. Chem. Phys. **139**(20), 204105 (2013). <https://doi.org/10.1063/1.4834596>
30. S. Bubin, M. Pavanello, W.C. Tung, K.L. Sharkey, L. Adamowicz, Chem. Rev. **113**(1), 36–79 (2013). <https://doi.org/10.1021/cr200419d>
31. M. Formanek, K.L. Sharkey, N. Kirnosov, L. Adamowicz, J. Chem. Phys. **141**(15), 154103 (2014). <https://doi.org/10.1063/1.4897634>
32. K.L. Sharkey, L. Adamowicz, J. Chem. Phys. **140**(17), 174112 (2014). <https://doi.org/10.1063/1.4873916>
33. E.A. Hylleraas, Z. Phys. **48**, 469 (1928)
34. E.A. Hylleraas, Z. Phys. **54**, 347 (1929)
35. F.W. King, D. Quicker, J. Langer, J. Chem. Phys. **134**, 124114 (2011). <https://doi.org/10.1063/1.3569565>
36. P.M. Kozłowski, L. Adamowicz, J. Chem. Phys. **95**, 6681 (1991). <https://doi.org/10.1063/1.461538>
37. P.M. Kozłowski, L. Adamowicz, J. Chem. Phys. **96**, 9013 (1992). <https://doi.org/10.1063/1.462259>
38. W. Cencek, J. Rychlewski, J. Chem. Phys. **98**, 1252 (1993)
39. W. Cencek, J. Rychlewski, J. Chem. Phys. **102**, 2533 (1995)
40. K. Varga, Y. Suzuki, Phys. Rev. C **52**, 2885 (1995)
41. Y. Suzuki, K. Varga, *Stochastic variational Approach to Quantum-Mechanical Few-Body Problems*, vol. 172 (Springer, New York, 1998)
42. D. Blume, Y. Yan, Phys. Rev. Lett. **113**, 213201 (2014). <https://doi.org/10.1103/PhysRevLett.113.213201>
43. M. Puchalski, K. Pachucki, Phys. Rev. Lett. **111**, 243001 (2013). <https://doi.org/10.1103/PhysRevLett.111.243001>
44. M. Puchalski, K. Pachucki, Phys. Rev. A **89**, 032510 (2014). <https://doi.org/10.1103/PhysRevA.89.032510>
45. M. Puchalski, K. Pachucki, Phys. Rev. A **92**, 012513 (2015). <https://doi.org/10.1103/PhysRevA.92.012513>
46. X.Y. Yin, D. Blume, Phys. Rev. A **92**, 013608 (2015). <https://doi.org/10.1103/PhysRevA.92.013608>
47. W.C. Tung, M. Pavanello, L. Adamowicz, J. Chem. Phys. **133**(12), 124106 (2010). <https://doi.org/10.1063/1.3491029>
48. S. Bubin, L. Adamowicz, J. Chem. Phys. **128**, 114107 (2008). <https://doi.org/10.1063/1.2894866>
49. K.L. Sharkey, M. Pavanello, S. Bubin, L. Adamowicz, Phys. Rev. A **80**, 062510 (2009). <https://doi.org/10.1103/PhysRevA.80.062510>
50. K.L. Sharkey, S. Bubin, L. Adamowicz, J. Chem. Phys. **134**, 044120 (2011). <https://doi.org/10.1063/1.3523348>
51. K.L. Sharkey, S. Bubin, L. Adamowicz, J. Chem. Phys. **134**, 194114 (2011). <https://doi.org/10.1063/1.3591836>
52. K.L. Sharkey, S. Bubin, L. Adamowicz, Phys. Rev. A **83**, 012506 (2011). <https://doi.org/10.1103/PhysRevA.83.012506>
53. K.L. Sharkey, S. Bubin, L. Adamowicz, J. Chem. Phys. **132**, 184106 (2010). <https://doi.org/10.1063/1.3419931>
54. Y. Suzuki, W. Horiuchi, M. Orabi, K. Arai, Few-Body Systems **42**(1–4), 33–72 (2008). <https://doi.org/10.1007/s00601-008-0200-3>
55. E. Mátyus, M. Reiher, J. Chem. Phys. **137**(2), 024104 (2012). <https://doi.org/10.1063/1.4731696>
56. K. Strasburger, J. Chem. Phys. **141**(4), 044104 (2014). <https://doi.org/10.1063/1.4890373>
57. M. Cafiero, S. Bubin, L. Adamowicz, Phys. Chem. Chem. Phys. **5**, 1491–1501 (2003). <https://doi.org/10.1039/B211193D>
58. J. Mitroy, S. Bubin, W. Horiuchi, Y. Suzuki, L. Adamowicz, W. Cencek, K. Szalewicz, J. Komasa, D. Blume, K. Varga, Rev. Mod. Phys. **85**, 693 (2013). <https://doi.org/10.1103/RevModPhys.85.693>
59. P.M. Kozłowski, L. Adamowicz, J. Chem. Phys. **97**, 5063 (1992). <https://doi.org/10.1063/1.463827>
60. J. Komasa, W. Cencek, J. Rychlewski, Phys. Rev. A **52**, 4500 (1995)
61. T. Joyce, K. Varga, J. Chem. Phys. **144**(18), 184106 (2016). <https://doi.org/10.1063/1.4948708>