Few-body problem in terms of correlated Gaussians

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In their textbook, Suzuki and Varga [*Stochastic Variational Approach to Quantum-Mechanical Few-Body Problems* (Springer, Berlin, 1998)] present the stochastic variational method with the correlated Gaussian basis in a very exhaustive way. However, the Fourier transform of these functions 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 formulas. We also give a derivation for formulations concerning central potentials.

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I. INTRODUCTION

Several different technical methods exist 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 nonorthogonal bases [5]. Each technics 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 us to consider very large bases with a minimum of variational effort. The drawback of this method is the nonorthogonality of basis wave functions with the possibility of appearance of spurious states due to overcompleteness; if this last inconvenience is overcome, using nonorthogonal 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 the time.

The stochastic variational method is described in full details in the remarkable textbook by Suzuki and Varga [5], where most important and fundamental formulas are derived. This very complete work will be referred 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 textbook. 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 formulas that are of crucial importance for some applications. In addition to the relativistic kinetic energy, we also derive 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 make our notations precise, and to have a self-contained paper, we will also present some formulas from SV. However, in order to separate what is new and what is already known, we relegate in appendixes all the formulas that can be found in SV, giving their reference number precisely. We will derive expressions for the most general correlated Gaussians (arbitrary number of particles $N+1$, arbitrary angular momentum L) but we restrict ourselves here to operators that do not mix spatial and spin degrees of freedom, so that we are concerned only with the matrix elements for 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). We focus on expressions for central potentials, the Fourier transform of correlated Gaussians, and its application to relativistic kinetic energy that are the subject of Secs. III–V. In the appendixes, we give the matrix elements for the overlap, the nonrelativistic kinetic energy, and an expression for central potentials. As already explained, except for special points, most of these formulas can be found in SV.

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 ($N \geqslant 1$). The particle i is located at P_i, so that the position vector relative to some origin O is $\boldsymbol{OP}_i=\boldsymbol{r}_i$, and has a corresponding conjugate momentum $\boldsymbol{p}_i$. 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 $\boldsymbol{R}_{\text{c.m.}}=\boldsymbol{x}_{N+1}$ and the corresponding total momentum $\boldsymbol{P}=\boldsymbol{\pi}_{N+1}$.

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The intrinsic description is expressed in terms 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 $m_{12,\ldots,i}=m_1+m_2+\cdots+m_i$ and G_i the center-of-mass of the first i particles: $\boldsymbol{OG}_i=(m_1\boldsymbol{r}_1+m_2\boldsymbol{r}_2+\cdots+m_i\boldsymbol{r}_i)/m_{12,\ldots,i}$. The Jacobi coordinate $\boldsymbol{x}_i$ is defined as the position of the particle $i+1$ relative to the center-of-mass G_i of the previous particles. Explicitly

$$\boldsymbol{x}_i=\boldsymbol{OG}_i-\boldsymbol{r}_{i+1}. \tag{1}$$

There are obviously N Jacobi coordinates $\boldsymbol{x}_i$ $(i\leqslant N)$ corresponding to intrinsic coordinates and the special vector $\boldsymbol{x}_{N+1}$ corresponds, as already mentioned, to the center-of-mass coordinate for the system (this vector has a physical meaning for particles with nonvanishing 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 Sec. V).

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

$$\boldsymbol{x}_i=\sum_{j=1}^{N+1}U_{ij}\boldsymbol{r}_j. \tag{2}$$

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

$$U_{ij}=\frac{m_j}{m_{12,\ldots,i}}\ \text{if}\ j\leqslant i,$$

$$U_{ii+1}=-1,$$

$$U_{ij}=0\ \text{if}\ j>i+1. \tag{3}$$

The inversion of relation (2) is often useful

$$\boldsymbol{r}_i=\sum_{j=1}^{N+1}(U^{-1})_{ij}\boldsymbol{x}_j. \tag{4}$$

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

$$(U^{-1})_{kl}=\frac{m_{l+1}}{m_{12,\ldots,l+1}},\quad k\leqslant l\leqslant N,$$

$$(U^{-1})_{l+1l}=-\frac{m_{12,\ldots,l}}{m_{12,\ldots,l+1}},\quad l\leqslant N,$$

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

$$(U^{-1})_{kN+1}=1\quad \forall\, k. \tag{5}$$

The conjugate momentum for variable $\boldsymbol{x}_i$ is denoted $\boldsymbol{\pi}_i=-i\partial/\partial\boldsymbol{x}_i$ $(\hbar=1)$ and must fulfill the conditions $[(\boldsymbol{x}_i)_k,(\boldsymbol{\pi}_j)_l]=i\delta_{ij}\delta_{kl}$. It is easy to check that the relations corresponding to Eqs. (2)–(4) are written

$$\boldsymbol{\pi}_i=\sum_{j=1}^{N+1}(U^{-1})_{ji}\boldsymbol{p}_j, \tag{6}$$

$$\boldsymbol{p}_i=\sum_{j=1}^{N+1}U_{ji}\boldsymbol{\pi}_j. \tag{7}$$

With this definition, the total momentum $\boldsymbol{P}=\boldsymbol{p}_1+\boldsymbol{p}_2+\cdots+\boldsymbol{p}_{N+1}$ is just $\boldsymbol{\pi}_{N+1}$.

B. Correlated Gaussians

In the stochastic variational method, the wave function for the system is expanded on Gaussian-type functions. Several different types of such basis states exist. 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 limited, because each pair of particles is in a S state. A more elaborated version considers instead the argument of the exponential as a bilinear combination of the Jacobi coordinates $\Sigma_{i,j=1}^{N}A_{ij}\boldsymbol{x}_i\cdot\boldsymbol{x}_j$. The matrix A must be symmetric $(A=\tilde{A})$ and positive definite. Obviously, the Hilbert space is enlarged and the convergence is accelerated.

To deal with a nonvanishing total angular momentum, one must introduce spherical harmonics somehow or other. The most elegant manner is to use a single solid harmonic $\mathcal{Y}_{LM}(\boldsymbol{v})=v^L Y_{LM}(\hat{v})$. 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 $\boldsymbol{v}=\Sigma_{i=1}^{N}u_i\boldsymbol{x}_i$.

In order to simplify the notations, let us introduce a "super vector" $\tilde{\boldsymbol{x}}=(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_N)$ 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 us 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),

$$\sum_{i,j=1}^{N}A_{ij}\boldsymbol{x}_i\cdot\boldsymbol{x}_j=\tilde{\boldsymbol{x}}\cdot A\boldsymbol{x},$$

$$\sum_{i=1}^{N}u_i\boldsymbol{x}_i=\tilde{u}\boldsymbol{x}. \tag{8}$$

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)

$$f_{KLM}(u,A;\boldsymbol{x})=\exp(-\tilde{\boldsymbol{x}}\cdot A\boldsymbol{x})|\tilde{u}\boldsymbol{x}|^{2K}\mathcal{Y}_{LM}(\tilde{u}\boldsymbol{x}). \tag{9}$$

The correlated Gaussian represents the basis state in coordinate representation $f_{KLM}(u,A;\boldsymbol{x})=\langle\boldsymbol{x}|\,\psi_{KLM}(u,A)\rangle$. Thus each

basis state is described by $N(N+3)/2$ free parameters [$N(N+1)/2$ for the matrix A and N for the vector u]. This prescription (9) is only able to deal with natural parity states. The term $|\tilde{u}\boldsymbol{x}|^{2K}$ is introduced for generality and to treat with more accuracy potentials with specific singular features. However, it complicates 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, $\langle\psi_{K'L'M'}(u',A')|\hat{O}|\psi_{KLM}(u,A)\rangle$. The crucial point in the computation of such an 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 Sec. VI C) for rigorous proofs.

Let us define the functions

$$g(\boldsymbol{s},A;\boldsymbol{x}) = \exp(-\tilde{\boldsymbol{x}}\cdot A\boldsymbol{x} + \tilde{\boldsymbol{s}}\cdot\boldsymbol{x}), \tag{10}$$

where $\boldsymbol{s}$ is an arbitrary super vector, $\tilde{\boldsymbol{s}}=(\boldsymbol{s}_1,\boldsymbol{s}_2,\ldots,\boldsymbol{s}_N)$, and, as usual, $\tilde{\boldsymbol{s}}\cdot\boldsymbol{x}=\Sigma_{i=1}^{N}\boldsymbol{s}_i\cdot\boldsymbol{x}_i$.

The g functions are called the generating functions for the correlated Gaussians since one has

$$f_{KLM}(u,A;\boldsymbol{x}) = \frac{1}{B_{KL}}\int d\hat{\boldsymbol{e}}\,Y_{LM}(\hat{\boldsymbol{e}}) \times\left(\frac{\partial^{2K+L}}{\partial\lambda^{2K+L}}g(\lambda\boldsymbol{e}u,A;\boldsymbol{x})\right)_{\lambda=0,|\boldsymbol{e}|=1}, \tag{11}$$

where the geometrical coefficient B_{KL} is defined as

$$B_{KL} = \frac{4\pi(2K+L)!}{2^K K!(2K+2L+1)!!}. \tag{12}$$

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

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

$$\langle\psi_{K'L'M'}(u',A')|\hat{O}|\psi_{KLM}(u,A)\rangle = \frac{1}{B_{K'L'}B_{KL}}\int d\hat{\boldsymbol{e}}d\hat{\boldsymbol{e}}\,Y_{LM}(\hat{\boldsymbol{e}})Y^{*}_{L'M'}(\hat{\boldsymbol{e}}) \times\left(\frac{\partial^{2K'+L'+2K+L}}{\partial\lambda'^{2K'+L'}\partial\lambda^{2K+L}}\langle O\rangle\right)_{\lambda=\lambda'=0,|\boldsymbol{e}|=|\boldsymbol{e}'|=1}. \tag{13}$$

with the matrix element between the generating function

$$\langle O\rangle = \langle g(\lambda'\boldsymbol{e}'u',A';\boldsymbol{x})|\hat{O}|g(\lambda\boldsymbol{e}u,A;\boldsymbol{x})\rangle. \tag{14}$$

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 nonvanishing elements are those with $L=L'$ and $M=M'$. Moreover, the matrix elements do not depend on the magnetic quantum number M.

III. CENTRAL POTENTIALS

In this section we present formulas for the matrix elements of a central potential; the corresponding expressions are more efficient for a numerical treatment than those presented in SV. For the definition of some dynamical quantities (i.e., $q,q',\rho,c,\gamma,\gamma',\ldots$) the reader is invited to have a look at Appendixes A and C.

Let us remark that the relationship (C6) gives a link between $\boldsymbol{e}\cdot\boldsymbol{e}'$ and the variable z. This opportunity allows us to put the exponential (C4) in the form

$$\exp[\bar{q}\lambda^2 + \bar{q}'\lambda'^2 + \rho c^2 z^2/(2\gamma\gamma')] \tag{15}$$

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 $i_0(cr|z|)\exp(-\bar{c}z^2/2)$ with the already mentioned relation (C5). The rest of the derivation is essentially similar to that of Appendix C. 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 similar to

$$\langle\psi_{K'LM}(u',A')|V(|\tilde{w}\boldsymbol{x}|)|\psi_{KLM}(u,A)\rangle = \frac{(2K'+L)!(2K+L)!}{B_{K'L}B_{KL}}\left(\frac{\alpha\pi^N}{\det B}\right)^{3/2} \times\sum_{n=0}^{K+K'+L}\left(\frac{\alpha}{2c}\right)^n J(n,\alpha,c) \times\sum_{k=0}^{\min(K,K')}\frac{2^{2k+L}}{(2k+L)!}B_{kL}F_{n,k}^{K,K',L}(\bar{q},\bar{q}',\gamma,\gamma'). \tag{16}$$

In this formula, the dynamical quantities c,γ,γ' are identical to those defined in Eq. (C9) while new quantities are necessary

$$\bar{q} = q - \frac{\rho\gamma}{2\gamma'},\quad \bar{q}' = q' - \frac{\rho\gamma'}{2\gamma},\quad \alpha = 1 - \frac{\rho c}{\gamma\gamma'}. \tag{17}$$

The form of the potential appears explicitly through the integral

$$J(n,\alpha,c) = \frac{1}{\sqrt{\pi}(2n+1)!} \times \int_0^\infty V(x\sqrt{2\alpha/c}) e^{-\alpha x^2} H_1(x) H_{2n+1}(x) dx. \tag{18}$$

Lastly, the geometrical function F is defined by

$$F_{n,k}^{K,K',L}(x,x',y,y') = n! \sum_{m=\max(k+L,n-K')}^{\min(n-k,K+L)} \frac{x^{K+L-m}}{(K+L-m)!} \times \frac{x'^{K'-n+m}}{(K'-n+m)!} \frac{y^{2m-L} y'^{2(n-m)+L}}{(m-k-L)!(n-k-m)!}. \tag{19}$$

Comparison between equivalent forms (C8), given in SV, and Eq. (16) warrants some comments.

They both have a very similar aspect. The form requires the calculations of three 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 this version; indeed the F function depends on four variables instead of five, it requires a single summation instead of a double, and the general monome needs one less factorial.

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

$$\frac{1}{a(a^2-1)^L} \int_0^\infty f(y) e^{-y^2} H_1(y) H_{2L+1}(ay) dy = \sum_{n=0}^{L} \left(\frac{a^2}{a^2-1}\right)^n \frac{(2L+1)!}{(L-n)!(2n+1)!} \times \int_0^\infty f(y) e^{-y^2} H_1(y) H_{2n+1}(y) dy \tag{20}$$

valid for any function $f(y)$.

The symmetry properties are more transparent in the SV version, but they can be proved as well in this version. Once the equivalence between both is shown this point is of minor importance. This version is especially interesting in the peculiar case $K=K'=0$ since the result writes

$$\langle \psi_{0LM} | V(|\tilde{w}\boldsymbol{x}|) | \psi_{0LM} \rangle = \mathcal{N}_L L! \left(\frac{\alpha}{1-\alpha}\right)^L \alpha^{3/2} J(L,\alpha,c), \tag{21}$$

where $\mathcal{N}_L$ is the overlap defined in Eq. (A5). In this case, there is no summation at all.

To finish this part, let us derive the general formula expressed in term of the $\mathcal{F}$ integral [see Eq. (C13)] instead of the J integral. The calculation relies essentially on the technics presented in Appendix C. The result is

$$\langle \psi_{K'LM}(u',A') V(|\tilde{w}\boldsymbol{x}|) | \psi_{KLM}(u,A) \rangle = \frac{4(2K'+L)!(2K+L)!}{\sqrt{\pi} B_{K'L} B_{KL}} \left(\frac{c\pi^N}{2 \det B}\right)^{3/2} \times \sum_{n=0}^{K+K'+L} \frac{\mathcal{F}_V(2n+2,c/2)}{(2n+1)!} \times \sum_{k=0}^{\min(K,K')} \frac{2^{2k+L}}{(2k+L)!} B_{kL} G_{n,k}^{K,K',L}(\bar{q},\bar{q}',\gamma,\gamma',c) \tag{22}$$

with function G defined by

$$G_{n,k}^{K,K',L}(\bar{q},\bar{q}',\gamma,\gamma',c) = \sum_{r=k+L}^{K+L} \frac{\bar{q}^{K+L-r} \bar{q}'^{K'+r-n} \gamma^{2r-L} \gamma'^{2(n-r)+L}}{(K+L-r)!(r-k-L)!} M_{n,k,r}^{K'} \left(-\frac{\alpha\gamma'^2}{2c\bar{q}'}\right) \tag{23}$$

and with

$$M_{n,k,r}^{K'}(z) = \sum_{s=\max(0,k+r-n)}^{K'+r-n} \frac{(s+n)!}{(K'+r-s-n)!(s+n-k-r)!} \frac{z^s}{s!}. \tag{24}$$

This formulation is also more efficient numerically than Eq. (C14) for the same reasons as those explained above. Application of this formula to the special case $K=K'=0$ leads exactly to the formula (C17) obtained before.

IV. 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

$$(2\pi)^{-3/2} \int e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} e^{-\alpha r^2} r^{2K} \mathcal{Y}_{LM}(\boldsymbol{r}) d\boldsymbol{r}. \tag{25}$$

The first thing to do is to use the traditional development of a plane wave in terms of spherical harmonics $e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} = 4\pi \Sigma_{l=0}^{\infty} (-i)^l j_l(qr) \Sigma_{m=-l}^{+l} Y_{lm}(\hat{\boldsymbol{q}}) Y_{lm}^*(\hat{\boldsymbol{r}})$, where $j_l(z) = \sqrt{\pi/(2z)} J_{l+1/2}(z)$ is the spherical Bessel function. Integration over angular $\hat{\boldsymbol{r}}$ variables leads to a $\delta_{lm,LM}$ 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 in the form $\int_0^\infty e^{-x^2} x^{2K+L+3/2} J_{L+1/2}(qx/\sqrt{\alpha})$. Fortunately, this integral is analytical and can be expressed in terms of generalized Laguerre polynomial L_n^a. This miraculous formula can be found in Ref. [6] [formula (6.631)]; it is written (it can be obtained

using the generating function of Laguerre polynomials expressed in term of Bessel functions [7])

$$\int_0^\infty e^{-x^2} x^{2n+\mu+1} J_\mu(2x\sqrt{z})dx = \frac{n!}{2} e^{-z} z^{\mu/2} L_n^\mu(z). \quad (26)$$

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

$$\frac{1}{(2\pi)^{3/2}} \int e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} e^{-\alpha r^2} r^{2K} \mathcal{Y}_{LM}(\boldsymbol{r})d\boldsymbol{r} = \frac{K!}{\alpha^K} L_K^{L+1/2}\left(\frac{q^2}{4\alpha}\right) \frac{(-i)^L}{(2\alpha)^{L+3/2}} e^{-q^2/(4\alpha)} \mathcal{Y}_{LM}(\boldsymbol{q}). \quad (27)$$

To get the formula corresponding to $K=0$, it is sufficient to replace in Eq. (27) 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

$$h_{0LM}(u,A;\pi) = (2\pi)^{-3N/2} \int e^{-i\tilde{\pi}\cdot\boldsymbol{x}} f_{0LM}(u,A;\boldsymbol{x})d\boldsymbol{x} = (2\pi)^{-3N/2} \int e^{-\tilde{\boldsymbol{x}}\cdot A\boldsymbol{x} - i\tilde{\pi}\cdot\boldsymbol{x}} \mathcal{Y}_{LM}(\tilde{u}\boldsymbol{x})d\boldsymbol{x} = I. \quad (28)$$

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

$$I = (2\pi)^{-3N/2} (\det A)^{-3/2} \int dz \exp(-\tilde{z}\cdot z - i\tilde{\pi}\cdot TD^{-1/2}z)\mathcal{Y}_{LM}(\tilde{u}TD^{-1/2}z). \quad (29)$$

In a second step, we change again from z to new $\boldsymbol{Z}$ variables with the help of an orthogonal matrix $U: \boldsymbol{Z}=Uz$. The Jacobian of the transformation is unity and, moreover, $\tilde{z}\cdot z = \tilde{\boldsymbol{Z}}\cdot\boldsymbol{Z}$. 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 $\boldsymbol{Z}_1$. Now, the integral takes the form

$$I = (2\pi)^{-3N/2} \alpha^{-L} (\det A)^{-3/2} \int d\boldsymbol{Z} \exp(-\tilde{\boldsymbol{Z}}\cdot\boldsymbol{Z} - i\tilde{\boldsymbol{V}}\cdot\boldsymbol{Z})\mathcal{Y}_{LM}(\boldsymbol{Z}_1) \quad (30)$$

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

Since the integral is separable for each variable, the rest of the proof is quite easy. $N-1$ integrals, corresponding to $\boldsymbol{Z}_k, k>1$ are equal to

$$(2\pi)^{-3/2} \int d\boldsymbol{Z}_k \exp(-\boldsymbol{Z}_k^2 - i\boldsymbol{V}_k\cdot\boldsymbol{Z}_k) = 2^{-3/2} \exp(-\boldsymbol{V}_k^2/4) \quad (31)$$

while the integral relative to $\boldsymbol{Z}_1$ can be calculated using expression (27) to get

$$(2\pi)^{-3/2} \int d\boldsymbol{Z}_1 \exp(-\boldsymbol{Z}_1^2 - i\boldsymbol{V}_1\cdot\boldsymbol{Z}_1)\mathcal{Y}_{LM}(\boldsymbol{Z}_1) = \frac{(-i)^L}{2^{L+3/2}} \exp(-\boldsymbol{V}_1^2/4)\mathcal{Y}_{LM}(\boldsymbol{V}_1). \quad (32)$$

Grouping all the exponentials into a single one gives an exponential with the argument $-(\boldsymbol{V}_1^2+\boldsymbol{V}_2^2+\cdots\boldsymbol{V}_N^2)/4 = -(\tilde{\boldsymbol{V}}\cdot\boldsymbol{V})/4 = -(\tilde{\pi}\cdot A^{-1}\pi)/4$. Thus, the final result for the FT looks similar to

$$h_{0LM}(u,A;\pi) = \frac{(-i)^L e^{-(1/4)\tilde{\pi}\cdot A^{-1}\pi}}{2^{L+3N/2}(\det A)^{3/2}} \mathcal{Y}_{LM}(\tilde{u}A^{-1}\pi). \quad (33)$$

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

$$h_{0LM}(u,A;\pi) = \frac{(-i)^L}{2^{L+3N/2}(\det A)^{3/2}} f_{0LM}\left(A^{-1}u, \frac{A^{-1}}{4}; \pi\right). \quad (34)$$

With this relationship, it is instructive to check the conservation of the norm, namely, $\mathcal{N}_L = \langle f_{0LM}|f_{0LM}\rangle = \langle h_{0LM}|h_{0LM}\rangle$.

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

$$h_{KLM}(u,A;\pi) = \langle\pi|\psi_{KLM}(u,A)\rangle = (2\pi)^{-3N/2} \int e^{-i\tilde{\pi}\cdot\boldsymbol{x}} f_{KLM}(u,A;\boldsymbol{x})d\boldsymbol{x} = (2\pi)^{-3N/2} \int e^{-\tilde{\boldsymbol{x}}\cdot A\boldsymbol{x} - i\tilde{\pi}\cdot\boldsymbol{x}} |\tilde{u}\boldsymbol{x}|^{2K} \mathcal{Y}_{LM}(\tilde{u}\boldsymbol{x})d\boldsymbol{x}. \quad (35)$$

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 $\boldsymbol{Z}_1$ variable that must be done now with help of the most general formula (27).

The FT for the general correlated Gaussian takes the form

$$h_{KLM}(u,A;\pi) = \frac{(-i)^L K!(\tilde{u}A^{-1}u)^K}{2^{L+3N/2}(\det A)^{3/2}} \times L_K^{L+1/2}\left(\frac{(\tilde{u}A^{-1}\pi)^2}{4\tilde{u}A^{-1}u}\right) e^{-(1/4)\tilde{\pi}\cdot A^{-1}\pi} \mathcal{Y}_{LM}(\tilde{u}A^{-1}\pi). \quad (36)$$

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

$$L_n^a(z) = \sum_{m=0}^{n} (-1)^m \frac{\Gamma(n+a+1)}{(n-m)!\Gamma(m+a+1)} \frac{z^m}{m!}, \tag{37}$$

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

$$h_{KLM}(u,A;\pi) = \frac{(-i)^L}{(2^{3N/2}\det A)^{3/2}} \sum_{K'=0}^{K} \frac{(-1)^{K'}K!}{K'!(K-K')!} \times \frac{(2K+2L+1)!!}{(2K'+2L+1)!!} \frac{(\tilde{u}A^{-1}u)^{K-K'}}{2^{K+K'+L}} \times f_{K'LM}\left(A^{-1}u, \frac{A^{-1}}{4}; \pi\right). \tag{38}$$

V. RELATIVISTIC KINETIC ENERGY

In many cases, the potential, or any operator, depends on the momenta $\pi_i = -i\partial/\partial \boldsymbol{x}_i$. If this dependence occurs through an integer power of the momenta, the method explained for example in Sec. II B, 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 $\tilde{w}\pi$. Then the calculation of the matrix element

$$\langle \psi_{K'LM}(u',A')|\hat{O}|\psi_{KLM}(u',A')\rangle = \langle h_{K'LM}(u',A';\pi)|\hat{O}(\tilde{w}\pi)|h_{KLM}(u,A;\pi)\rangle$$

can be performed using the expansion (38). The dynamical element to be calculated has a form similar to

$$\left\langle f_{K'LM}\left(A'^{-1}u', \frac{A'^{-1}}{4}; \pi\right) \middle| \hat{O}(\tilde{w}\pi) \middle| f_{KLM}\left(A^{-1}u, \frac{A^{-1}}{4}; \pi\right) \right\rangle. \tag{39}$$

This last element is then computed by application of Eq. (16) [or Eq. (C8)] with the trivial changes $u \to A^{-1}u$, $A \to A^{-1}/4$, $u' \to A'^{-1}u'$, $A' \to A'^{-1}/4$.

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

$$T_R = \sum_{i=1}^{N+1} \sqrt{\boldsymbol{p}_i^2 + m_i^2}. \tag{40}$$

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 $\boldsymbol{P} = \boldsymbol{0}$ in the subsequent formulas. In particular, the momentum $\boldsymbol{p}_i$ relative to the particle i writes [see relation (7)]

$$\boldsymbol{p}_i = \sum_{j=1}^{N} U_j^{(i)} \pi_j = \tilde{U}^{(i)}\pi \tag{41}$$

with

$$U_j^{(i)} = 0 \quad \text{if } j < i-1,$$

$$U_j^{(i)} = -1 \quad \text{if } j = i-1,$$

$$U_j^{(i)} = \frac{m_i}{m_{12\cdots j}} \quad \text{if } j \geqslant i. \tag{42}$$

In order to present simple formulas, let us focus on the special case $K=K'=0$. Then

$$\langle \psi_{0LM}(u',A')|T_R|\psi_{0LM}(u,A)\rangle = \sum_{i=1}^{N+1} \langle h_{0LM}(u',A';\pi)|\sqrt{|\tilde{U}^{(i)}\pi|^2 + m_i^2}|h_{0LM}(u,A;\pi)\rangle. \tag{43}$$

The computation of the matrix element in the summation is performed first using Eq. (34) and then Eq. (C17) with the appropriate parameters.

The final result looks similar to

$$\langle \psi_{0LM}(u',A')|T_R|\psi_{0LM}(u,A)\rangle = \frac{\mathcal{N}_L}{\sqrt{4\pi}} \sum_{i=1}^{N+1} Z_i^{-3/2} \sum_{n=0}^{L} \frac{L!}{2^n(2n+1)!(L-n)!} \times \mathcal{F}\left(2n+2, \frac{1}{4Z_i}, m_i\right) \left(\frac{\gamma_i\gamma_i'}{\rho}\right)^n \left(1 - \frac{Z_i\gamma_i\gamma_i'}{2\rho}\right)^{L-n}. \tag{44}$$

Again, the matrix element is proportional to the overlap $\mathcal{N}_L$. The ρ parameter is defined as in formula (A4) while

$$Z_i = \tilde{U}^{(i)}A'B^{-1}AU^{(i)}, \quad \gamma_i = \frac{\tilde{U}^{(i)}A'B^{-1}u}{Z_i},$$

$$\gamma_i' = \frac{\tilde{U}^{(i)}AB^{-1}u'}{Z_i}, \tag{45}$$

and the integral for the potential is given by

$$\mathcal{F}(k,A,m) = \int_0^\infty du e^{-Au^2} u^k \sqrt{u^2+m^2}. \tag{46}$$

In fact, we need in Eq. (44), the values of $\mathcal{F}(k,A,m)$ for even values of $k \geqslant 2$. We calculated this function in the following way. Let us define for simplicity $\mathcal{I}_l = \mathcal{F}(2l+2,A,m)$ and introduce the parameter $\beta = Am^2/2$. The first values can be found analytically

$$\mathcal{I}_0 = \frac{1}{2A^2}\beta e^\beta K_1(\beta), \tag{47a}$$

$$\mathcal{I}_1 = \frac{1}{2A^3}\beta e^\beta [\beta K_0(\beta) + (2-\beta)K_1(\beta)], \tag{47b}$$

where $K_n(z)$ is the modified Bessel function. The integral for higher l can be obtained by the following recursion formula;

$$\mathcal{I}_l = \frac{1}{A}\mathcal{I}_{l-1} + \frac{(2l-1)(l+1-2\beta)}{A^2}\mathcal{I}_{l-2}. \tag{48}$$

All the above formulas allow us 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.

VI. CONCLUDING REMARKS

In this paper, we propose a number of formulas 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 formulas relative to central potentials. Instead of integrals containing Hermite polynomials, we proposed formulas 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 formulas can be simplified a lot in the special case $K=K'=0$.

However, 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 formulas 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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APPENDIX A: OVERLAP

The overlap between basis states $\mathcal{N}_{K'KL} = \langle \psi_{K'LM}(u',A') | \psi_{KLM}(u,A) \rangle$ is a crucial ingredient in the equation of motion. Since the basis states are nonorthogonal, 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. Explicitly, one finds (see SV, Table 7.1 p. 124):

$$\langle g(\boldsymbol{s}',A';\boldsymbol{x}) | g(\boldsymbol{s},A;\boldsymbol{x}) \rangle = \left(\frac{\pi^N}{\det B}\right)^{3/2} \exp\left(\frac{1}{4}\tilde{\boldsymbol{v}}\cdot B^{-1}\boldsymbol{v}\right) = \mathcal{M}_0, \tag{A1}$$

where

$$B = A + A', \ \boldsymbol{v} = \boldsymbol{s} + \boldsymbol{s}'. \tag{A2}$$

The overlap is obtained introducing result (A1) in the general formula (13). Since the variables $\lambda, \lambda', \hat{\boldsymbol{e}}, \hat{\boldsymbol{e}}'$ appear only in $\boldsymbol{v}$, the term depending on $\det B$ factorizes out the integral. The exponential is then expanded as a series in $\lambda, \lambda', \boldsymbol{e}\cdot\boldsymbol{e}'$. The derivation and integration are performed without difficulty. The final result is [SV, Eq. (A6), p. 248]

$$\mathcal{N}_{K'KL} = \frac{(2K'+L)!(2K+L)!}{B_{K'L}B_{KL}}\left(\frac{\pi^N}{\det B}\right)^{3/2} \times \sum_{k=0}^{\min(K,K')} B_{kL}\frac{q^{K-k}}{(K-k)!}\frac{q'^{K'-k}}{(K'-k)!}\frac{\rho^{2k+L}}{(2k+L)!} \tag{A3}$$

with the following complementary definitions:

$$q = \frac{1}{4}\tilde{u}B^{-1}u, \quad q' = \frac{1}{4}\tilde{u}'B^{-1}u',$$

$$\rho = \frac{1}{2}\tilde{u}'B^{-1}u = \frac{1}{2}\tilde{u}B^{-1}u'. \tag{A4}$$

For the important peculiar case $K'=K=0$, this formula simplifies a lot and we are left with [SV, Eq. (A7), p. 249]:

$$\mathcal{N}_{00L} = \mathcal{N}_L = \frac{(2L+1)!!}{4\pi}\left(\frac{\pi^N}{\det B}\right)^{3/2}\rho^L. \tag{A5}$$

APPENDIX B: NONRELATIVISTIC KINETIC ENERGY

It is well known that the use of Jacobi coordinates allows us to share the total kinetic energy operator $T = \sum_{i=1}^{N+1} \boldsymbol{p}_i^2/(2m_i)$ into the kinetic energy of the system as a bulk $T_{\text{c.m.}} = \boldsymbol{P}^2/(2M)$ $(M = m_{12,\ldots,N+1})$ and an intrinsic kinetic energy operator T_{NR} depending only on intrinsic momenta.

A simple calculation leads to the explicit expression

$$T_{\text{NR}} = T - T_{\text{c.m.}} = \frac{1}{2}\sum_{i,j=1}^{N} \Lambda_{ij}\boldsymbol{\pi}_i\cdot\boldsymbol{\pi}_j = \frac{1}{2}\tilde{\boldsymbol{\pi}}\cdot\Lambda\boldsymbol{\pi}, \tag{B1}$$

where the supervector $\tilde{\boldsymbol{\pi}} = (\boldsymbol{\pi}_1, \boldsymbol{\pi}_2, \ldots, \boldsymbol{\pi}_N)$ is introduced. The matrix Λ is symmetric and its general element writes

$$\Lambda_{ij} = \sum_{k=1}^{N+1} U_{ik}U_{jk}\frac{1}{m_k}. \tag{B2}$$

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, p. 124):

$$\langle g(\boldsymbol{s}',A';\boldsymbol{x}) | \tilde{\boldsymbol{\pi}}\cdot\Lambda\boldsymbol{\pi} | g(\boldsymbol{s},A;\boldsymbol{x}) \rangle = \mathcal{M}_0[6\text{Tr}(AB^{-1}A'\Lambda) - \tilde{\boldsymbol{y}}\cdot\Lambda\boldsymbol{y}], \tag{B3}$$

where $\mathcal{M}_0$ is precisely the overlap expression (A1), $\text{Tr}(X)$ means the trace of the X matrix, and the supervector $\boldsymbol{y}$ is given by

$$\boldsymbol{y} = A'B^{-1}\boldsymbol{s} - AB^{-1}\boldsymbol{s}'. \tag{B4}$$

It remains to insert result (B3) into Eq. (13). The variables $\lambda,\lambda',\boldsymbol{e}\cdot\boldsymbol{e}'$ appear now still in the exponential part of $\mathcal{M}_0$ but also in $\tilde{\boldsymbol{y}}\cdot\Lambda\boldsymbol{y}$ 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, Eq. (A10), p. 250]

$$\begin{aligned}&\langle\psi_{K'LM}(u',A')|\tilde{\pi}\cdot\Lambda\pi|\psi_{KLM}(u,A)\rangle\\&= \frac{(2K'+L)!(2K+L)!}{B_{K'L}B_{KL}}\left(\frac{\pi^N}{\det B}\right)^{3/2}\sum_{k=0}^{\min(K,K')} B_{kL}[Rqq'\rho\\&\quad + P(K-k)q'\rho + P'(K'-k)q\rho + Q(2k+L)qq']\\&\quad\times\frac{q^{K-k-1}}{(K-k)!}\frac{q'^{K'-k-1}}{(K'-k)!}\frac{\rho^{2k+L-1}}{(2k+L)!}\end{aligned} \tag{B5}$$

with the numbers P,P',Q,R defined by

$$P = -\tilde{u}B^{-1}A'\Lambda A'B^{-1}u, \quad P' = -\tilde{u}'B^{-1}A\Lambda AB^{-1}u',$$

$$Q = 2\tilde{u}'B^{-1}A\Lambda A'B^{-1}u, \quad R = 6\mathrm{Tr}(AB^{-1}A'\Lambda). \tag{B6}$$

Again, the formula for the special case $K=K'=0$ is much simpler:

$$\langle\psi_{0LM}(u',A')|\tilde{\pi}\cdot\Lambda\pi|\psi_{0LM}(u,A)\rangle = \mathcal{N}_L\left(R + L\frac{Q}{\rho}\right). \tag{B7}$$

The pleasant feature is the factorization of the overlap matrix.

Clearly the matrix $\tilde{U}$, transpose of U defined in Eq. (3), is different from U^{-1} defined in Eq. (5). Thus U is not an orthogonal matrix. Nevertheless, one has the property $\det U = 1$. This matrix has also another very interesting property.

Let us define the reduced mass μ_i for particle i by

$$\frac{1}{\mu_i} = \frac{1}{m_{12,\ldots,i}} + \frac{1}{m_{i+1}}. \tag{B8}$$

It can be shown that the definition (2) allows one to write the nonrelativistic kinetic energy operator in a form without mixed terms, namely,

$$T_{\mathrm{NR}} = \frac{1}{2}\tilde{\pi}\cdot\Lambda\pi = \sum_{i=1}^{N}\frac{\pi_i^2}{2\mu_i}. \tag{B9}$$

This means that, in the matrix elements (B5)–(B7), one can restrict the calculations to a diagonal matrix Λ since, in this case, $\Lambda_{ij}=(1/\mu_i)\delta_{ij}$.

APPENDIX C: CENTRAL POTENTIALS

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 $V=\Sigma_i V_i(\boldsymbol{r}_i - R_{\mathrm{c.m.}})$ while in the second situation the potential has a form $V=\Sigma_{i<j}V_{ij}(\boldsymbol{r}_i-\boldsymbol{r}_j)$. This is the consequence of translational invariance. In both cases, the argument of any potential is always a linear combination of Jacobi coordinates, so that the most general form of the potential is a sum of terms such as $V(\tilde{w}\boldsymbol{x})$.

In this case, one can write generally

$$\langle\psi|V(\tilde{w}\boldsymbol{x})|\psi\rangle = \int V(\boldsymbol{r})\langle\psi|\delta^3(\tilde{w}\boldsymbol{x}-\boldsymbol{r})|\psi\rangle d\boldsymbol{r}. \tag{C1}$$

It is necessary to calculate the matrix elements of $\delta(\tilde{w}\boldsymbol{x}-\boldsymbol{r})$ on the generating functions; these are given in SV, Table 7.1, p. 124.

However, we are interested here in central potentials that are also invariant under rotations; the argument of the potential must be now $|\tilde{w}\boldsymbol{x}|$. Although it is possible to work with Eq. (C1) imposing a scalar potential $V(r)=V(|\boldsymbol{r}|)$, it is preferable to impose this property from the very beginning and replace the three-dimensional integral (C1) by the following one-dimensional integral:

$$\langle\psi|V(|\tilde{w}\boldsymbol{x}|)|\psi\rangle = \int V(r)\langle\psi|\delta(|\tilde{w}\boldsymbol{x}|-r)|\psi\rangle dr. \tag{C2}$$

It is necessary to calculate the matrix elements of $\delta(|\tilde{w}\boldsymbol{x}|-r)$ 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 $\delta^3(\tilde{w}\boldsymbol{x}-\boldsymbol{r})$ in spherical coordinates and integrating on angular variables. We find

$$\begin{aligned}&\langle g(\boldsymbol{s}',A';\boldsymbol{x})|\delta(|\tilde{w}\boldsymbol{x}|-r)|g(\boldsymbol{s},A;\boldsymbol{x})\rangle\\&= \frac{4\mathcal{M}_0}{\sqrt{\pi}}\times\frac{r^2}{(\tilde{w}B^{-1}w)^{3/2}}i_0\left(\frac{r|\tilde{w}B^{-1}\boldsymbol{v}|}{\tilde{w}B^{-1}w}\right)\\&\quad\times\exp\left(-\frac{r^2+(\tilde{w}B^{-1}\boldsymbol{v})^2/4}{\tilde{w}B^{-1}w}\right),\end{aligned} \tag{C3}$$

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

One must implement the element (C3) into Eq. (13). For further convenience, we give here more information concerning this computation. Let us note $c=2/(\tilde{w}B^{-1}w)$. 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 $\lambda,\lambda',\boldsymbol{e}\cdot\boldsymbol{e}'$ are present in the exponential part of $\mathcal{M}_0$ which is explicitly written

$$\mathcal{M}_0 \propto \exp(q\lambda^2 + q'\lambda'^2 + \rho\lambda\lambda'\boldsymbol{e}\cdot\boldsymbol{e}'). \tag{C4}$$

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

$$i_0(Bz)\exp(-Az^2) = \frac{\sqrt{A}}{B}\sum_{n=0}^{\infty}\frac{(Az^2)^n}{(2n+1)!}H_{2n+1}(B/2\sqrt{A}). \tag{C5}$$

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

$$(c^2\boldsymbol{z}^2)^n = (\gamma^2\lambda^2 + \gamma'^2\lambda'^2 + 2\gamma\gamma'\lambda\lambda'\boldsymbol{e}\cdot\boldsymbol{e}')^n \tag{C6}$$

which must be maintained in the derivation and which is expanded as a series. It is gathered with the series coming from exponential (C4). After this grouping, the general monome of this series has the form $\lambda^s\lambda'^{s'}(\boldsymbol{e}\cdot\boldsymbol{e}')^t$. The derivation $\partial^{2K+L}/\partial\lambda^{2K+L}$ being taken for $\lambda=0$ leads to a term $(2K+L)!\delta_{2K+L,s}$; one also has a term $(2K'+L)!\delta_{2K'+L,s'}$ coming from the derivation with respect to λ'. Lastly, the term $(\boldsymbol{e}\cdot\boldsymbol{e}')^t$ is expanded as (do not forget that $|\boldsymbol{e}|=1=|\boldsymbol{e}'|$)

$$(\boldsymbol{e}\cdot\boldsymbol{e}')^t = 4\pi\sum_{lm}\frac{t!}{(t-l)!!(t+l+1)!!}Y^*_{lm}(\hat{\boldsymbol{e}})Y_{lm}(\hat{\boldsymbol{e}}) \tag{C7}$$

and the integration over $\hat{\boldsymbol{e}}$ and $\hat{\boldsymbol{e}}'$ leads to a term $B_{kL}\delta_{2k+L,t}$.

After this tedious but straightforward cooking, and using expression (C2), we get the final result [SV, Eq. (A.128), p. 282]

$$\begin{aligned}\langle\psi_{K'LM}(u',A')|V(|\tilde{w}\boldsymbol{x}|)|\psi_{KLM}(u,A)\rangle &= \left(\frac{\pi^N}{\det B}\right)^{3/2}\frac{(2K'+L)!(2K+L)!}{B_{K'L}B_{KL}}\sum_{n=0}^{K+K'+L}\frac{J(n,c)}{c^n} \\ &\times \sum_{k=0}^{\min(K,K')} B_{kL}F^n_{K-k,K'-k,2k+L}(q,q',\rho,\gamma,\gamma').\end{aligned} \tag{C8}$$

In this formula, the dynamical quantities q,q',ρ are defined in Eq. (A4) for the overlap, while the new ones c,γ,γ' are specific to the potential

$$c = \frac{2}{\tilde{w}B^{-1}w}, \quad \gamma = \frac{\tilde{w}B^{-1}u}{\tilde{w}B^{-1}w}, \quad \gamma' = \frac{\tilde{w}B^{-1}u'}{\tilde{w}B^{-1}w}. \tag{C9}$$

The form of the potential appears explicitly through the integral

$$J(n,c) = \frac{1}{\sqrt{\pi}(2n+1)!}\int_0^{\infty}V(x\sqrt{2/c})e^{-x^2}H_1(x)H_{2n+1}(x)dx. \tag{C10}$$

Lastly, the geometrical function F is defined as

$$\begin{aligned}F^n_{p,p',l}(q,q',\rho,\gamma,\gamma') &= n!\sum_{m,m'}\frac{q^{p-m}}{(p-m)!}\frac{q'^{p'-m'}}{(p'-m')!} \\ &\times \frac{\rho^{l-n+m+m'}}{(l-n+m+m')!}\frac{\gamma^{n+m-m'}\gamma'^{n-m+m'}}{2^{m+m'}m!m'!(n-m-m')!}.\end{aligned} \tag{C11}$$

We tried to express this function in term 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 (C8) has a nice property that allows 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, ρ and c remain unchanged. The symmetry follows from the property $F^n_{p,p',l}(q,q',\rho,\gamma,\gamma') = F^n_{p',p,l}(q',q,\rho,\gamma',\gamma)$. 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 $n=0$, $J(n,c)/c^n=1$, $F^0_{p,p',l}=q^pq'^{p'}\rho^l/[p!p'!l!]$, 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, Eq. (A.130), p. 282]

$$\langle\psi_{0LM}|V(|\tilde{w}\boldsymbol{x}|)|\psi_{0LM}\rangle = \mathcal{N}_L L!\sum_{n=0}^{L}\frac{J(n,c)}{(L-n)!}\left(\frac{\gamma\gamma'}{\rho c}\right)^n. \tag{C12}$$

Here again, the overlap factorizes.

A small drawback in the formulas (C8) and (C12) is the presence of the Hermite polynomial $H_{2n+1}(x)$. One way to deal with it is the use of recursion formulas. 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

$$\mathcal{F}_V(k,A) = \int_0^{\infty}V(u)u^ke^{-Au^2}du. \tag{C13}$$

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 expres-

sion for the matrix elements in terms of $\mathcal{F}_V$ functions. This form is absent in SV:

$$\langle \psi_{K'LM}(u',A')|V(|\tilde{w}\boldsymbol{x}|)|\psi_{KLM}(u,A)\rangle = \frac{(2K'+L)!(2K+L)!}{\sqrt{2\pi}2^{K+K'-1}B_{K'L}B_{KL}}\left(\frac{c\pi^N}{\det B}\right)^{3/2}\frac{\gamma^{2K+L}\gamma'^{2K'+L}}{(-c)^{K+K'+L}} \times \sum_{n=0}^{K+K'+L}\frac{(-2c)^n\mathcal{F}_V(2n+2,c/2)}{(2n+1)!}\sum_{k=0}^{\min(K,K')}4^k B_{kL} \times H_{n,k}^{K,K',L}\left(\frac{2q\gamma'}{\rho\gamma},\frac{2q'\gamma}{\rho\gamma'},\frac{\rho c}{\gamma\gamma'}\right) \tag{C14}$$

with function H defined by

$$H_{n,k}^{K,K',L}(x,x',y) = \sum_{r=0}^{K+K'+L-n}(-1)^r \times \frac{(K+K'+L-r)!y^r}{(K+K'+L-n-r)!}G_{k,r}^{K,K',L}(x,x') \tag{C15}$$

and

$$G_{k,r}^{K,K',L}(x,x') = \sum_{s=0}^{K-k}\sum_{s'=0}^{K'-k}\frac{x^s x'^{s'}}{s!(K-k-s)!s'!(K'-k-s')!} \times \frac{1}{(r-s-s')!(2k+L+s+s'-r)!}. \tag{C16}$$

Due to the property $G_{k,r}^{K,K',L}(x,x')=G_{k,r}^{K',K,L}(x',x)$ the hermiticity of the element is transparent.

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

$$\langle \psi_{0LM}(u',A')|V(|\tilde{w}\boldsymbol{x}|)|\psi_{0LM}(u,A)\rangle = \mathcal{N}_L 2c\sqrt{\frac{c}{2\pi}}L!\times\sum_{n=0}^{L}\frac{2^n\mathcal{F}_V(2n+2,c/2)}{(2n+1)!(L-n)!} \times\left(\frac{\gamma\gamma'}{\rho}\right)^n\left(1-\frac{\gamma\gamma'}{\rho c}\right)^{L-n}. \tag{C17}$$

This formula needs essentially the same numerical effort than expression (C12) but it is written in terms of a much more convenient integral.

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