Exact solution for two-dimensional Coulomb matrix elements

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Exact analytic expression is derived for the matrix elements of the Coulomb interaction in two dimensions in the form of a closed finite sum expression. The orthonormal complete set of eigenfunctions of the harmonic oscillator \(|n_xn_y\rangle\) is used as the basis for spanning real space. Several recurrence relations have been found in order to simplify the task of calculating the usually vast amount of elements required for any computer simulation.

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The choice of the anisotropic orthonormal complete set of eigenfunctions of the harmonic oscillator is due to the ubiquity and special symmetric properties of this particular problem in the field of quantum mechanics. The projection of this basis into real space is

\[
\langle xy | n_xn_y \rangle = \psi_{n_xn_y}(x,y) = \left( \frac{1}{a_xa_y} \right)^{1/2} \left( \frac{1}{2^{n_x}n_x!2^{n_y}n_y!} \right)^{1/2} e^{-\frac{x^2}{a_x^2}} e^{-\frac{y^2}{a_y^2}} H_{n_x}(x/a_x) e^{-\frac{x^2}{a_x^2}} H_{n_y}(y/a_y),
\]

\[
\langle n'_x n'_y | n_xn_y \rangle = \delta_{n_xn'_x} \delta_{n_xn'_y},
\]

Without any loss of generality we can assume that

\[
a_x > a_y.
\]

Just the case \(a_x = a_y\) will fall apart from our supposition. There is no problem in treating this case apart, as it is even simpler to calculate and can be derived from our results. The eccentricity parameter \(\gamma\) is defined as

\[
\gamma = \frac{a_y}{a_x},
\]

\[
0 < \gamma < 1.
\]

It is of great interest to express the wavefunctions and Coulomb potential as their two-dimensional Fourier transforms

\[
\psi_\lambda(r) = \frac{1}{2\pi} \int \phi_\lambda(q)e^{-iq\cdot r} dq,
\]

\[
V(r) = \frac{1}{2\pi} \int \tilde{V}(q)e^{-iq\cdot r} dq.
\]

Under this notation, the matrix elements take a different expression

\[
\mathcal{V}_{\lambda_1\lambda_2}^{\lambda_3\lambda_4} = \frac{1}{2\pi} \int \phi_{\lambda_1}^*(q_1)\phi_{\lambda_2}(q_1 - q)\phi_{\lambda_3}(q_2)\phi_{\lambda_4}(q_2 + q)\tilde{V}(q)dq_1dq_2dq,
\]

where \(\lambda_i\) represents the set of quantum numbers \(\{n'_x, n'_y\}\) for the \(i\)-th particle.

\[
\mathcal{V}_{\lambda_1\lambda_2}^{\lambda_3\lambda_4} = \frac{1}{2\pi} \int C_{\lambda_1\lambda_3}(q)D_{\lambda_2\lambda_4}(q)\tilde{V}(q)dq,
\]

where

\[
C_{\lambda_1}(q) = \int \phi_{\lambda_1}^*(k)\phi_{\lambda_1'}(k - q) dk = \int \psi_{\lambda_1}(r)\psi_{\lambda_1'}(r)e^{-iqr} dr,
\]

\[
D_{\lambda_2}(q) = \int \phi_{\lambda_2}^*(k)\phi_{\lambda_2'}(k + q) dk = \int \psi_{\lambda_2}(r)\psi_{\lambda_2'}(r)e^{iqr} dr
\]

\[
= C_{\lambda_2}(-q).
\]
The calculation of $C_{\lambda' \lambda}(q)$ is quite straightforward. It can be separated in both two dimensions, as they are (almost) symmetrical. The calculation proceeds as follows (normalization constants omitted for clarity)

$$
\int_{-\infty}^{\infty} e^{-x^2/2} H_{n_1^+}(x/a_x) H_{n_2^+}(x/a_x) e^{-iq_x x} \, dx = a_x \int_{-\infty}^{\infty} e^{-x'^2/2} H_{n_1^+}(x') H_{n_2^+}(x') e^{-iq_x x'} \, dx'
= a_x \int_{-\infty}^{\infty} e^{-x'^2/2} H_{n_1^+}(x') H_{n_2^+}(x') e^{-iq_x x'} \, dx',
$$

(12)

where $x' = a_x x$ and $q'_x = a_x q_x$. This equation can be seen as the Fourier transform of the product of two functions:

$$
\mathcal{F}[f_{n_1^+} f_{n_2^+}],
$$

(13)

being

$$
f_n(x) = e^{-x^2/2} H_n(x).
$$

(14)

Making use of the properties of the Fourier transform, in particular the one that states that the transform of the product of two functions is the convolution of their transforms, i.e.

$$
\mathcal{F}[f g] = \mathcal{F}[f] * \mathcal{F}[g].
$$

(15)

In our particular case, the Fourier transform of the function $f_n(x)$ has a very simple form as it is an eigenfunction of this operator with associated eigenvalue $i^n$:

$$
\mathcal{F}[f_n(x)](q_x) = i^n f_n(q_x).
$$

(16)

It only remains now to calculate the convolution product, defined as

$$
f * g = \int_{-\infty}^{\infty} f(t) g(t - \tau) \, d\tau = \int_{-\infty}^{\infty} g(\tau) f(t - \tau) \, d\tau.
$$

(17)

In our case, we have to calculate the following integral

$$
\mathcal{F}[f_{n_1^+} f_{n_2^+}] = i^{n_1^+ + n_2^+} \int_{-\infty}^{\infty} e^{-x'^2/2} H_{n_1^+}(x') e^{-(q'_x - x')^2/2} H_{n_2^+}(q'_x - x') \, dx'.
$$

(18)

Let us first do the following change of variables:

$$
\begin{align*}
x' &= u + q'_x / 2 & q'_x &= 2x' - 2u \\
dx' &= du & (-\infty, \infty) & \rightarrow & (-\infty, \infty).
\end{align*}
$$

(19)

Thus, choosing $n_{1+}^{14} = \max(n_1^+, n_2^+)$ and $n_{1-}^{14} = \min(n_1^+, n_2^+)$, the last integral is transformed to

$$
\int_{-\infty}^{\infty} e^{-(u+q'_x/2)^2/2} H_{n_{1+}^{14}}(u + q'_x/2) e^{-(q'_x - u - q'_x/2)^2/2} H_{n_{1-}^{14}}(q'_x - u - q'_x/2) \, du
= e^{-q'_x^2/4} \int_{-\infty}^{\infty} e^{-u^2} H_{n_{1+}^{14}}(u + q'_x/2)(-1)^{n_{1+}^{14}} H_{n_{1-}^{14}}(u - q'_x/2) \, du,
$$

(20)

which according to Gradshteyn & Ryzhik Eq. 7.377 in page 797

$$
\int_{-\infty}^{\infty} e^{-x^2} H_m(x+y) H_n(x+z) \, dx = 2^n \pi^{1/2} m! z^{-m} L^{n-m}_{m}(-2yz) [m \leq n],
$$

(21)

the result of integral (20) is

$$
2^{n_{1+}^{14} + n_{1-}^{14}} \left( \frac{a_x q_x}{2} \right)^{n_{1+}^{14} - n_{1-}^{14}} L^{n_{1+}^{14} - n_{1-}^{14}}_{n_{1-}^{14}}(a_x^2 q_x^2/2).
$$

(22)
Collecting all terms together, we can write the final result for $C(q)$:

$$C^{n_x \cdot n_y}_{n_x \cdot n_y}(q_x, q_y) = \left( \frac{1}{a_x a_y \pi} \right) \left( \frac{1}{2n_x^{1/4}} \frac{1}{2n_y^{1/4}} \frac{1}{2n_x^{1/4}} \frac{1}{2n_y^{1/4}} \right)^{1/2} \int_{n_x^{1/4} + n_y^{1/4} + n_x^{1/4}}^{n_x^{1/4} + n_y^{1/4} + n_x^{1/4}} a_x a_y 2n_x^{14} 2n_y^{14} \pi n_x^{14} n_y^{14} \frac{1}{(-1)^{n_x^{1/4} + n_y^{1/4}}} e^{-a_x^2 q_x^2/4} \left( - \frac{a_x q_x}{2} \right)^{n_x^{1/4} - n_x^{1/4}} \left( \frac{a_y q_y}{2} \right)^{n_y^{1/4} - n_y^{1/4}} e^{-a_y^2 q_y^2/4} \left( - \frac{a_y q_y}{2} \right)^{n_y^{1/4} - n_y^{1/4}} (a_x q_x^2/2) (a_y q_y^2/2) \right)^{1/2} \int_{n_x^{1/4} + n_y^{1/4} + n_x^{1/4}}^{n_x^{1/4} + n_y^{1/4} + n_x^{1/4}} L_{n_x^{1/4} - n_x^{1/4}}^{n_x^{1/4} - n_x^{1/4}} (a_x q_x^2/2) L_{n_y^{1/4} - n_y^{1/4}}^{n_y^{1/4} - n_y^{1/4}} (a_y q_y^2/2).$$

In the same fashion we calculate the function $D$:

$$D^{n_x \cdot n_y}_{n_x \cdot n_y}(q_x, q_y) = (-1)^{n_x^{1/2} + n_y^{1/2}} \left( \frac{1}{2n_x^{1/4}} \frac{1}{2n_y^{1/4}} \frac{1}{2n_x^{1/4}} \frac{1}{2n_y^{1/4}} \right)^{1/2} \int_{n_x^{1/4} + n_y^{1/4} + n_x^{1/4}}^{n_x^{1/4} + n_y^{1/4} + n_x^{1/4}} a_x a_y 2n_x^{23} 2n_y^{23} \pi n_x^{23} n_y^{23} \frac{1}{(-1)^{n_x^{1/4} + n_y^{1/4}}} e^{-a_x^2 q_x^2/4} \left( - \frac{a_x q_x}{2} \right)^{n_x^{23} - n_x^{23}} \left( \frac{a_y q_y}{2} \right)^{n_y^{23} - n_y^{23}} e^{-a_y^2 q_y^2/4} \left( - \frac{a_y q_y}{2} \right)^{n_y^{23} - n_y^{23}} (a_x q_x^2/2) (a_y q_y^2/2) \right)^{1/2} \int_{n_x^{23} + n_y^{23} + n_x^{23}}^{n_x^{23} + n_y^{23} + n_x^{23}} L_{n_x^{23} - n_x^{23}}^{n_x^{23} - n_x^{23}} (a_x q_x^2/2) L_{n_y^{23} - n_y^{23}}^{n_y^{23} - n_y^{23}} (a_y q_y^2/2).$$

The Fourier transform of the Coulombic potential is

$$\tilde{V}(q) = \int_0^\infty V(r) J_0(rq) r \, dr = \xi \frac{1}{q} = \xi \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-(q_x^2 + q_y^2)u^2} \, du$$

$$= \xi \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-(a_x^2 q_x^2 + a_y^2 q_y^2)u^2/a_x^2} \, du$$

$$= \xi a_x \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-(q_x^2 + q_y^2)u^2/\gamma^2} \, du$$

$$V(r) = \frac{\xi}{r}.$$  

Where we have substituted the dimensionless momentum variables,

$$q_x' = a_x q_x;$$
$$q_y' = a_y q_y.$$  

The integration can be now performed. Making use of the expansion of the Laguerre polynomials as

$$L_{n}^{l}(x) = \sum_{k=0}^{n} \left( \begin{array}{c} (-1)^{k} \frac{1}{k!} \left( \frac{n + l}{n - k} \right) \end{array} \right) x^{k},$$

let us focus on the $q_x$ and $q_y$ dependent part. Let us also forget about any multiplicative constants and summation.
indices, we can write the matrix element as:

\[
\mathcal{V}_{n_x n_y n_{x'} n_{y'}} = \frac{1}{2\pi} (-1)^{n_{x'} + n_{x} - n_{y} + n_{y'}} \left( \frac{2n_{x'} n_{x}! n_{y}! n_{y'}!}{n_{x}! n_{x'}! n_{y}! n_{y'}!} \right)^{1/2} (-1)^{s_x + s_y + n_{x'} + n_{x} - n_{y} + n_{y'}}
\]

\[
\xi \alpha x \frac{2}{\sqrt{\pi}} \sum_{k_x=0}^{n_{x'}} (-1)^{k_x} \left( \frac{n_{x}!}{n_{x} - k_x!} \right) \sum_{k_{x'}=0}^{n_{x'}} (-1)^{k_{x'}} \left( \frac{n_{x'}!}{n_{x'} - k_{x'}!} \right) \sum_{k_y=0}^{n_{y'}} (-1)^{k_y} \left( \frac{n_{y}!}{n_{y} - k_y!} \right) \sum_{k_{y'}=0}^{n_{y'}} (-1)^{k_{y'}} \left( \frac{n_{y'}!}{n_{y'} - k_{y'}!} \right)
\]

\[
\left( \frac{1}{2} \right)^{s_x + s_y + k_x + k_{x'} + k_y + k_{y'}} \int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} \frac{dq'_x}{aq_x} e^{-(u^2 + 1/2)q'_x^2} q'_x (2s_x + 2k_x + 2k_{x'}) \int_{-\infty}^{\infty} \frac{dq'_y}{aq_y} e^{-(u^2/\gamma^2 + 1/2)q'_y^2} q'_y (2s_y + 2k_y + 2k_{y'})
\]

(32)

The last three integrals can be solved quite easily. First, the ones depending in \( q'_x \) and \( q'_y \) lead to:

\[
\int_{-\infty}^{\infty} e^{-(u^2 + 1/2)q'_x^2} q'_x (2s_x + 2k_x + 2k_{x'}) \, dq'_x = 2^{a+1/2} \Gamma (a + 1/2) \left( 1 + 2u^2 \right)^{a+1/2}
\]

\[
\int_{-\infty}^{\infty} e^{-(u^2/\gamma^2 + 1/2)q'_y^2} q'_y (2s_y + 2k_y + 2k_{y'}) \, dq'_y = 2^{b+1/2} \Gamma (b + 1/2) \left( 1 + 2u^2/\gamma^2 \right)^{b+1/2}
\]

where \( a = s_x + k_x + k_{x'} \) and \( b = s_y + k_y + k_{y'} \). We have already included the condition for the integral to be non-zero:

\[
2s_x = |n_{x}^1 - n_{x}^4| + |n_{x}^2 - n_{x}^3| = n_{x}^1 - n_{x}^4 + n_{x}^2 - n_{x}^3,
\]

\[
2s_y = |n_{y}^1 - n_{y}^4| + |n_{y}^2 - n_{y}^3| = n_{y}^1 - n_{y}^4 + n_{y}^2 - n_{y}^3,
\]

\[
s_x, s_y \in \mathbb{N}.
\]

(37)

Now, the \( u \)-integration can be performed.

\[
\int_{0}^{\infty} \frac{1}{(1 + 2u^2/\gamma^2)^{b+1/2}} \frac{1}{(1 + 2u^2)^{a+1/2}} \, du = \frac{1}{2} \left( \frac{2}{\gamma^2} \right)^{-1/2} B \left( \frac{1}{2}, a + b + \frac{1}{2} \right) \times 2F1 \left( a + \frac{1}{2}, \frac{1}{2}; a + b + 1, 1 - \gamma^2 \right)
\]

(38)

which was solved with the help of Gradshteyn & Ryzhik Integral 3.259 3, page 326 (check also the errata)

\[
\int_{0}^{\infty} x^{\lambda - 1} (1 + \alpha x^p)^{-\mu} (1 + \beta x^p)^{-\nu} \, dx = \frac{1}{p} \alpha^{-1/p} B \left( \frac{\lambda}{p}, \mu + \nu - \frac{\lambda}{p} \right) 2F1 \left( \nu, \frac{\lambda}{p}; \mu + \nu; 1 - \beta \right)
\]

\[
|\arg \alpha| < \pi, \quad |\arg \beta| < \pi, \quad p > 0, \quad 0 < \Re \lambda < 2 \Re (\mu + \nu)
\]

(39)
Grouping all terms together, we end up with:

\[
\mathcal{V}^{n_x n_z n_x n_y} = \frac{1}{2\pi \xi} \frac{1}{\sqrt{2\pi}} (-1)^{s_x + s_y + n_x^2 + n_y^2 + n_x^3 + n_y^3} \left( \frac{n_x^{14} - n_y^{14} - n_{x_z}^{23} - n_{y_z}^{23}}{n_x^{14} + n_y^{14} + n_{x_z}^{23} + n_{y_z}^{23}} \right)^{1/2} \\
\sum_{k_x = 0}^{n_x^{14}} \frac{(-1)^{k_x}}{k_x!} \left( \frac{n_x^{14}}{n_x^{14} - k_x} \right) \sum_{k_x' = 0}^{n_x^{23}} \frac{(-1)^{k_x'}}{k_x'!} \left( \frac{n_x^{23}}{n_x^{23} - k_x'} \right) \Gamma(s_x + k_x + k_x' + \frac{1}{2}) \frac{1}{a_x a_y} 2F_1 \left( s_x + k_x + k_x' + \frac{1}{2} ; s_x + s_y + k_x + k_y + k_x' + k_y' + 1, 1 - \gamma^2 \right) .
\]

After some compactation we get the final result:

\[
\mathcal{V}^{n_x n_z n_x n_y} = \frac{1}{a_x \sqrt{2\pi}} (-1)^{s_x + s_y + n_x^2 + n_y^2 + n_x^3 + n_y^3} \left( \frac{n_x^{14} - n_y^{14} - n_{x_z}^{23} - n_{y_z}^{23}}{n_x^{14} + n_y^{14} + n_{x_z}^{23} + n_{y_z}^{23}} \right)^{1/2} \\
\sum_{k_x = 0}^{n_x^{14}} \frac{(-1)^{k_x}}{k_x!} \left( \frac{n_x^{14}}{n_x^{14} - k_x} \right) \sum_{k_x' = 0}^{n_x^{23}} \frac{(-1)^{k_x'}}{k_x'!} \left( \frac{n_x^{23}}{n_x^{23} - k_x'} \right) \Gamma(s_x + k_x + k_x' + \frac{1}{2}) \frac{1}{a_x a_y} 2F_1 \left( s_x + k_x + k_x' + \frac{1}{2} ; s_x + s_y + k_x + k_y + k_x' + k_y' + 1, 1 - \gamma^2 \right) .
\]

**RECURRENTE**

In order to optimize the computing times, let us try to find some recurrence relations for the kernel of the summation.

\[
v_{ij} = B \left( \frac{i}{2}, i + j + \frac{1}{2} \right) 2F_1 \left( i + \frac{1}{2}, \frac{1}{2}; i + j + 1; 1 - \gamma^2 \right) = B_{i+j} F_{i+j} .
\]

The Beta function behaves as follows

\[
B_0 = \pi , \quad B_k = \frac{k - \frac{1}{2}}{k} B_{k-1} .
\]
The Gauss hypergeometric function does it in a more complex way

\[
a(z-1)_{2}F_{1}(a+1,b;c;z) = (c-a)_{2}F_{1}(a-1,b;c;z) + (c-2a+(a-b)z)_{2}F_{1}(a,b;c;z) \quad (45)
\]

\[
0 = (c-1)_{2}F_{1}(a,b,c-1,z)
+ c(c-1+(a+b-2c+1)z)_{2}F_{1}(a,b,c,z)
+ (a-c)(b-c)zz_{2}F_{1}(a,b,c+1,z)
\quad (46)
\]

\[
_{2}F_{1}(a,b;c;z) = \frac{(c-1)(2-c-(a+b-2c+3)z)}{(a-c+1)(b-c+1)z} \quad (47)
\]

\[
_{2}F_{1}(a,b;c;z) = \frac{c-2a+2+(a-b-1)z}{(a-1)(z-1)} \quad (48)
\]

In our case \( a = k + \frac{1}{2}, \) \( b = \frac{1}{2} \) and \( c = l + 1. \) Therefore if \( F_{kl} = _2F_{1}(k+\frac{1}{2};\frac{1}{2};l+1;z): \)

\[
F_{kl} = \frac{l(l-1)(2+k-2l)z}{(\frac{1}{2}-l)(\frac{1}{2}+k-l)z} F_{k,l-1} - \frac{l(l-1)(1-z)}{(\frac{1}{2}-l)(\frac{1}{2}+k-l)z} F_{k,l-2}, \quad (49)
\]

\[
F_{kl} = \frac{2-2k+l+(k-1)z}{(k-\frac{1}{2})(z-1)} F_{k-1,l} - \frac{k-l-\frac{3}{2}}{(k-\frac{1}{2})(z-1)} F_{k-2,l}, \quad (50)
\]

where \( z = 1 - \gamma^2. \) Now combining expressions (44), (49) and (50), it is possible to find a recursive relation for the rows and columns of \( v_{ij}. \) For the columns:

\[
v_{ij} = B_{i+j}F_{i,i+j}
= \frac{i+j}{i+j} B_{i+j-1} \left( \frac{(i+j)(1-i-j-(2-i-2j)(1-\gamma^2))}{(j-\frac{1}{2})(i+j-\frac{1}{2})(1-\gamma^2)} F_{i,i+j-1} + \frac{(i+j-1)(i+j)\gamma^2}{(j-\frac{1}{2})(i+j-\frac{1}{2})(1-\gamma^2)} F_{i,i+j-2} \right)
= 1 - i - j - (2-i-2j)(1-\gamma^2) B_{i+j-1} F_{i,i+j-1} + \frac{(i+j-1)\gamma^2}{(j-\frac{1}{2})(1-\gamma^2)} B_{i+j-1} F_{i,i+j-2}
= 1 - i - j - (2-i-2j)(1-\gamma^2) v_{i,j-1} + \frac{(i+j-1)\gamma^2}{(j-\frac{1}{2})(1-\gamma^2)} i + j - \frac{3}{2} B_{i+j-2} F_{i,i+j-2}
= 1 - i - j - (2-i-2j)(1-\gamma^2) v_{i,j-1} + \frac{(i+j-\frac{3}{2})\gamma^2}{(j-\frac{1}{2})(1-\gamma^2)} v_{i,j-2}, \quad (51)
\]

And for the rows:

\[
v_{ij} = B_{i+j}F_{i,i+j}
= B_{i+j} \left( \frac{1+i+(1-i)\gamma^2}{(\frac{1}{2}-i)\gamma^2} F_{i-1,i+j} + \frac{(j+\frac{3}{2})}{(i-\frac{1}{2})\gamma^2} F_{i-2,i+j} \right)
= 1 + j + (1-i)\gamma^2 v_{i-1,j+1} + \frac{j+\frac{3}{2}}{(i-\frac{1}{2})\gamma^2} v_{i-2,j+2}. \quad (52)
\]
The diagram for the column iteration (with fixed row).

\[
\begin{array}{cccc}
& \cdots & j & \cdots \\
\vdots & \ddots & \ddots & \ddots \\
\vdots \end{array}
\]

\[
i \cdots \cdots \cdots v_{i,j-2} \quad v_{i,j-1} \quad v_{ij} \quad \bullet
\]

And for row iteration.

\[
\begin{array}{ccc}
\vdots & \ddots & \ddots \\
\vdots \end{array}
\]

\[
i \cdots \cdot v_{i-1,j+1}
\]

The seed for the iteration is:

| \(v_{ij}\) | 0 | 1 | 2 |
|---|---|---|---|
| 0 | \(2K(z)\) | \(\frac{2}{z}(E(z) + (z - 1)K(z))\) | \(\frac{2}{z}(2(z - 1)K(z) - (z - 2)E(z))\) |
| 1 | \(\frac{1}{z} (K(z) - E(z))\) | \(\frac{1}{z} (2(z - 1)K(z) - (z - 2)E(z))\) |
| 2 | \(\frac{1}{z} (2(z - 1)K(z) - (z - 2)E(z))\) |

NOTES

The Gamma function for half-integer values is defined as:

\[
\Gamma \left(n + \frac{1}{2}\right) = \frac{(2n-1)!!}{2^n} \sqrt{\pi}.
\]

(53)

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